Computational Chemistry in Parallel

by

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A thesis submitted in partial fulfillment of the requirements for the degree of

Master of Science.

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 \bigodot Dylan Hennessey, 2018

Abstract

General Purpose computing with Graphics Processing Units (GPGPU) is a method of computation that allows for calculations to be performed in parallel. Graphics Processing Units (GPU) allow a single basic computer to perform as well as a super computer cluster composed of only Central Processing Units (CPU), at a fraction of the cost. As quantum computational chemistry scales very poorly with the size of systems, the use of GPGPU has been a very effective tool for quantum chemists.

This thesis presents a program called cudaDFRATOM. This program, written in CUDA Fortran, allows for the calculation and optimization of Well-Tempered Basis Sets (WTBS) at the four-component relativistic level of theory. Except for a few small initial calculations and control flow, all work is performed entirely on the GPU.

When calculating the two-electron integrals, cudaDFRATOM uses a very effective method of utilizing as much of the GPU's resources as possible and can calculate these integrals approximately 20 times faster than a similar program running on only a CPU.

Two different algorithms for forming the \mathbf{P} and \mathbf{Q} supermatrices are presented. The relatively small size of these matrices and the need to use double-precision floating-point operations stunts the speedup of these algorithms such that they only attain a speedup of about 2 times over the CPU program. An overall speedup of about 4 times is achieved by cudaDFRATOM.

In addition, new WTBS are calculated for non-relativistic levels of theory using the rWTBS program and at the four-component relativistic level of theory using cudaDFRATOM. In both cases, a novel algorithm for automating the optimization of these basis sets was used. The algorithm finds a basis set that is as small a possible while still retaining sufficient accuracy to numerical calculations.

Preface

This thesis is my own original work. No part of this thesis has been previously published. Computations and code were planned, performed, and written by myself with the help of Mariusz Klobukowski.

In addition, I have also worked on a project with Mariusz which is not in this thesis. The project investigated how the FHF⁻ molecule behaves in a confining potential. The results were published in a paper titled "Hydrogen bonding and autoionization in confined bifluoride system FHF⁻" in *The Journal of Physics B: Atomic, Molecular and Optical Physics* vol. 50 page 155101 in the year 2017.

For Jessie, who puts up with more than she needs to

Acknowledgements

I would first like to acknowledge my supervisor, Mariusz Klobukowski. Few grad students are lucky enough to have a mentor who is as kind, helpful, and a source of as much interesting conversation as he. I would not have as easily discovered my love of programming if it weren't for him, and for that I am truly grateful. He dealt with my ... sporadic writing schedule with the patience and grace of a saint which made this whole process of writing a thesis that much more bearable. I really cannot say enough how much his guidance has meant to me.

I would like to thank one of my course instructors, Paul Lu. He took a chance with me when no one else would and gave me the opportunity to more fully explore my computational potential. I don't think I could have made it without his help, so again, thank you.

I would also like to thank my friends and family. As much as I love it, the science can't be the reason to wake up *every* morning, so thank you to those who helped keep my spirits up, especially when it seemed like I would be writing this forever.

I should also thank the money. The work in this thesis could not have happened without the funding from NSERC and FGSR, and without the computer resources of WestGrid and Compute Canada.

Finally, I would like to thank my girlfriend Jessie Hartmann. We've been through Hell and back together, and there is no one else I would have rather had at my side than her. For some reason, she continues to love me, even as I make her watch a video on sorting algorithms for the tenth time, so for you Jessie I give my appreciation, affection, and love.

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List of Symbols

Some symbols are reused. The exact meaning will need to be obtained from context.

Symbol	Description	
Ĥ	Hamiltonian operator	
Ψ	Wavefunction	
E	Energy	
∇	Gradient of a function	
\hat{H}_{el}	Electronic Hamiltonian operator	
a_o	Bohr radius	
ψ	Spin orbital	
ϕ	Orbital	
α	Spin function, four-component matrix, Gaussian nuclei exponent, well-tempered basis set parameter	
β	Spin function, four-component matrix, well-tempered basis set parameter	
ω	Spin coordinate	
ϵ	Vector of spin orbital energies	
Φ	Basis function	
ζ	Basis function exponent	
λ	Orbital symmetry	
μ	Orbital symmetry	
c	Speed of light	
m_0	Mass of object at rest	
\hbar	Reduced Planck's constant	
$q_{}$	Particle charge	
\hat{A},\hat{arphi}	Electromagnetic field potentials	
$oldsymbol{\psi}$	Large component spinor	
$oldsymbol{\phi}$	Small component spinor	
ϵ_0	Permittivity of free space	
δ	Well-tempered basis set parameter	
γ	Well-tempered basis set parameter	

Chapter 1 Introduction

Graphics Processing Units (GPUs) have allowed quantum chemists to overcome to problem of two-electron integral scaling[1–4]. This has allowed for very large systems to be studied at a very accurate level of chemical theory [5]. There has been little advancement in the relativistic levels of chemical theory however. Therefore, this thesis presents a program called cudaDFRATOM which allows for the optimization of basis sets at the Dirac-Fock-Roothaan level of theory. In this chapter, the background of relativistic theory is discussed. In Chapter 2, the details of the code used in cudaDFRATOM are given. Chapter 3 discusses the basis sets cudaDFRATOM produces.

1.1 Solving the Schrödinger Equation

The Schrödinger equation[6] in its time-independent, non-relativistic form is given in Equation 1.1

$$\hat{H}\Psi = E\Psi \tag{1.1}$$

where \hat{H} is the Hamiltonian operator, Ψ is referred to as the wavefunction, and E is the energy of the system described by the wavefunction. For a molecular system, the Hamiltonian operator in atomic units (a.u.) is given by Equation 1.2

$$\hat{H} = -\frac{1}{2} \sum_{i}^{n} \nabla_{i}^{2} - \sum_{A}^{N} \frac{1}{2M_{A}} \nabla_{A}^{2} - \sum_{i}^{n} \sum_{A}^{N} \frac{Z_{A}}{r_{iA}} + \sum_{i}^{n} \sum_{j>i}^{n} \frac{1}{r_{ij}} + \sum_{A}^{N} \sum_{B>A}^{N} \frac{Z_{A}Z_{B}}{r_{AB}}$$
(1.2)

where *i* and *j* refer to electrons, *A* and *B* refer to nuclei, and *n* and *N* refer to the maximum number of electrons and nuclei, respectively. M_A and Z_A are the mass and charge of nucleus *A*. r_{xy} is the distance between particles *x* and *y*, and $\nabla_n^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ where *x*, *y*, and *z* are the Cartesian coordinates of particle *n*. Each term accounts for a different kind

of energy: $-\frac{1}{2}\sum_{i}^{n} \nabla_{i}^{2}$ is the kinetic energy of the electrons, $\sum_{A}^{N} \frac{1}{2M_{A}} \nabla_{A}^{2}$ is the kinetic energy of the nuclei, $\sum_{i}^{n} \sum_{A}^{N} \frac{Z_{A}}{r_{iA}}$ is the potential energy of attraction between nuclei and electrons, $\sum_{i}^{n} \sum_{j>i}^{N} \frac{1}{r_{ij}}$ is the potential energy of repulsion between electrons, and $\sum_{A}^{N} \sum_{B>A}^{N} \frac{Z_{A}Z_{B}}{r_{AB}}$ is the potential energy of repulsion between nuclei. Together, this accounts for all of the energy of a molecular system. As this operator is quite complex, it would be helpful to simplify it if possible. Fortunately, Born and Oppenheimer[7] realized that an approximation could be made that would substantially reduce the amount of work we have to do.

Much like a satellite in orbit around the Earth, the proton and neutron vastly outweigh the electron. If we look at the second term in Equation 1.2, we notice that it is inversely proportional to the mass of the nuclei. We can therefore assume, to a decent approximation, that the kinetic energy of the nuclei is very close to zero compared to the other terms. This allows us to treat them as stationary classical particles. As a bonus, this turns the potential energy of repulsion between nuclei into a constant. This approximation reduces the Hamiltonian operator to the *electronic* Hamiltonian given in Equation 1.3

$$\hat{H}_{el} = -\frac{1}{2} \sum_{i}^{n} \nabla_{i}^{2} - \sum_{i}^{n} \sum_{A}^{N} \frac{Z_{A}}{r_{iA}} + \sum_{i}^{n} \sum_{j>i}^{n} \frac{1}{r_{ij}} + \sum_{B>A}^{N} \frac{Z_{A}Z_{B}}{r_{AB}}$$
(1.3)

 \hat{H} can be assumed to be \hat{H}_{el} for the remainder of this thesis, and with the Hamiltonian out of the way, we can now turn our attention to the wavefunction. While we were able to get away with turning nuclei into classical particles, the electrons unfortunately remain fully quantum. Therefore, we need to deal with all the complicated mathematical baggage this comes with.

Consider the hydrogen atom which, like all other one-electron atomic systems, is one of the few exactly solvable problems in quantum mechanics. The solution for its wavefunction in spherical coordinates is given in Equation 1.4[8]

$$\Psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_l^m(\theta,\varphi) \tag{1.4}$$

where R_{nl} is called the radial function and $Y_l^m(\theta, \varphi)$ is called the angular function. The radial function has the form

$$R_{nl}(r) = \frac{1}{r} \left(\frac{r}{a_o n}\right)^{l+1} e^{-\frac{r}{a_o n}} L_{n-l-1}^{2l+1} \left(\frac{r}{a_o n}\right)$$
(1.5)

where a_o is the Bohr radius and $L_{n-l-1}^{2l+1}\left(\frac{r}{a_o n}\right)$ is a Laguerre polynomial of $\left(\frac{r}{a_o n}\right)$ and order $j_{\max} = n - l - 1$ of $\left(\frac{r}{a_o n}\right)$. Its coefficients are given by

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}c_j \tag{1.6}$$

where c_0 is a constant determined by normalization. The polynomial itself given by

$$L_{q-p}^{p}(x) = (-1)^{p} \left(\frac{d}{dx}\right)^{q} L_{q}(x)$$
(1.7)

$$L_q(x) = e^x \left(\frac{d}{dx}\right)^q \left[x^q e^{-x}\right]$$
(1.8)

The angular function has the form

$$Y_l^m(\theta,\varphi) = \epsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} P_l^m(\cos\theta) e^{im\varphi}$$
(1.9)

where $i = \sqrt{-1}$ and $\epsilon = (-1)^m$ for $m \ge 0$ or 1 if m < 0. $P_l^m(\cos \theta)$ is a polynomial of $\cos \theta$ and has the form of

$$P_l^m(x) = (1 - x^2)^{\frac{|m|}{2}} \frac{d^{|m|}}{dx^{|m|}} P_l(x)$$
(1.10)

$$P_l(x) = \frac{1}{2^l l!} \frac{d^j}{dx^j} (x^2 - 1)^l$$
(1.11)

Inspection of these equations reveals that n must be a positive integer greater than 0, l must be a positive integer between 0 and n-1, and |m| can be no larger than l. The integers n, l, and m are called quantum numbers, specifically n is the principal quantum number, l is the azimuthal quantum number, and m is the magnetic quantum number. Notice that there is no limit to how large n can get, which suggests that there is not just one solution to this equation, but an infinite number of them. The hydrogen-like atom wavefunctions are given the special name of orbitals. Also, orbitals with the same value of l are referred to be of the same symmetry. Table 1.1 shows the reduced form of Ψ for a few different orbitals. For atoms with more than one electron, if we make a further assumption that electrons can be modelled like ideal springs, it has been shown that an atomic system with two electrons can also be solved[9], but we can go no further than this. At least, not exactly. In the next section we will see how solutions for atoms, and indeed molecules, can begin to be approached.

1.2 Hartree-Fock Method

While the wavefunction might appear complex, it is important to remember that it is still just a wave, and one of the fundamental properties of waves is that they can be added together to produce a separate, more complex wave. Likewise, any wave, no matter how complex, can be broken down as a summation of many simpler waves[10]. Thus, any linear combination

n	l		
_	0		1
	m = 0	m = 0	$m = \pm 1$
1	$\left(\frac{1}{\pi a_o^3}\right)^{\frac{1}{2}} e^{\left(-\frac{r}{a_o}\right)}$	_	_
2	$\frac{1}{\sqrt{8\pi a_o^3}} \left(1 - \frac{r}{2a_o}\right) e^{\left(-\frac{r}{2a_o}\right)}$	$\frac{1}{\sqrt{32\pi a_o^3}} \frac{r}{a_o} e^{\left(-\frac{r}{2a_o}\right)} \cos \theta$	$\mp \frac{1}{\sqrt{64\pi a_o^3}} \frac{r}{a_o} e^{\left(-\frac{r}{2a_o}\right)} \sin \theta e^{\pm i\varphi}$

 Table 1.1: The first few exact solutions for the hydrogen atom wavefunction.

of solutions to the Schrödinger equation must therefore be a solution of a different equation. It is this property that will be exploited to solve our many electron problem. But first we must define some ground rules.

The first rule is that the overall wavefunction must describe a system of fermions. This means that the wavefunction must be antisymmetric with respect to the exchanging of electronic coordinates, i.e. $\Psi(1, 2, ..., n, ..., m) = -\Psi(1, 2, ..., m, ..., n)$ and the probability density of the wavefunction must be indistinguishable with respect to the exchanging of electronic coordinates, i.e. $|\Psi(1, 2, ..., n, ..., m)|^2 = |\Psi(1, 2, ..., m, ..., n)|^2$. The easiest way to meet this requirement is by using a Slater determinant[11], and by introducing the concept of spin. Spin is a fourth quantum number, which we have neglected to talk about so far. Spin is a confusing property that some quantum particles have. No one really knows what it is, other than to say it has something to do with the angular momentum of the particle, and oddly enough that it in no way refers to the direction that the particle is spinning. It has been shown to have binary values[12], which will be refered to as up spin (\uparrow) and down spin (\downarrow). A Slater determinant that obeys antisymmetry is shown in Equation 1.12

$$\Psi(1,2,3,\ldots,n) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \psi_1(1) & \psi_2(1) & \psi_3(1) & \ldots & \psi_n(1) \\ \psi_1(2) & \psi_2(2) & \psi_3(2) & \ldots & \psi_n(2) \\ \psi_1(3) & \psi_2(3) & \psi_3(3) & \ldots & \psi_n(3) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \psi_1(n) & \psi_2(n) & \psi_3(n) & \ldots & \psi_n(n) \end{vmatrix}$$
(1.12)

Here, *n* refers to the number of electrons in the system, and the numbers in parentheses refer to specific electrons. ψ_i refers to the *i*th spin orbital which is equal to $\phi_{\frac{i+1}{2}}(r,\theta,\varphi)\alpha(\omega)$ if *i* is odd, or $\phi_{\frac{i}{2}}(r,\theta,\varphi)\beta(\omega)$ if *i* is even (ϕ is an orbital and ω is the spin coordinate). α and β are called spin functions. What they actually are doesn't matter, but they do have to be orthonormal to each other.

$$\langle \alpha(\omega_i) | \alpha(\omega_i) \rangle = \langle \beta(\omega_i) | \beta(\omega_i) \rangle = 1 \langle \alpha(\omega_i) | \beta(\omega_i) \rangle = \langle \beta(\omega_i) | \alpha(\omega_i) \rangle = 0$$
 (1.13)

Using Slater determinants has some interesting consequences. If we had a system where two electrons of the same spin were in the same spin orbital, that would mean that two of the columns would be equal to one another. Such a determinant would be equal to zero, which means that the wavefunction for such a system would not exist. This is the famous Pauli antisymmetry principle[13]. The math showing that it satisfies antisymmetry is shown below[14].

$$\Psi(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(1)\alpha(\omega_1) & \phi_1(1)\beta(\omega_1) \\ \phi_1(2)\alpha(\omega_2) & \phi_1(2)\beta(\omega_2) \end{vmatrix}$$
(1.14)

$$\Psi(1,2) = \frac{1}{\sqrt{2}} \left[\phi_1(1)\alpha(\omega_1)\phi_1(2)\beta(\omega_2) - \phi_1(1)\beta(\omega_1)\phi_1(2)\alpha(\omega_2) \right]$$
(1.15)

$$-\Psi(1,2) = \frac{1}{\sqrt{2}} \left[\phi_1(1)\beta(\omega_1)\phi_1(2)\alpha(\omega_2) - \phi_1(1)\alpha(\omega_1)\phi_1(2)\beta(\omega_2)\right]$$
(1.16)

$$-\Psi(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(2)\alpha(\omega_2) & \phi_1(2)\beta(\omega_2) \\ \phi_1(1)\alpha(\omega_1) & \phi_1(1)\beta(\omega_1) \end{vmatrix} = \Psi(2,1)$$
(1.17)

As can be seen, changing the indexing of the electrons is equivalent to swapping the rows for those electrons, which changes the sign of the determinant. It is important to note that because observable quantities depend not the wavefunction, but the *absolute square* of the wavefunction, altering the indexing of the electrons does not change the calculation of these observables. Consider the example of the electron density probability distribution shown below (note that ϕ , α , and β are real in this example, but even if they weren't the results would not change).

$$|\Psi(1,2)|^{2} = \frac{1}{2} \begin{bmatrix} \left| \phi_{1}(1)\alpha(\omega_{1}) & \phi_{1}(1)\beta(\omega_{1}) \right|^{2} \\ \phi_{1}(2)\alpha(\omega_{2}) & \phi_{1}(2)\beta(\omega_{2}) \end{bmatrix}^{2} \end{bmatrix}$$
(1.18)

$$|\Psi(1,2)|^{2} = \frac{1}{2} [(\phi_{1}(1)\alpha(\omega_{1})\phi_{1}(2)\beta(\omega_{2}) - \phi_{1}(1)\beta(\omega_{1})\phi_{1}(2)\alpha(\omega_{2})) \\ \times (\phi_{1}(1)\alpha(\omega_{1})\phi_{1}(2)\beta(\omega_{2}) - \phi_{1}(1)\beta(\omega_{1})\phi_{1}(2)\alpha(\omega_{2}))]$$
(1.19)

$$|\Psi(1,2)|^{2} = \frac{1}{2} \int \int \int \int [\phi_{1}(1)^{2} \alpha(\omega_{1})^{2} \phi_{1}(2)^{2} \beta(\omega_{2})^{2} + \phi_{1}(1)^{2} \beta(\omega_{1})^{2} \phi_{1}(2)^{2} \alpha(\omega_{2})^{2} - 2\phi_{1}(1)^{2} \alpha(\omega_{1}) \beta(\omega_{1}) \phi_{1}(2)^{2} \beta(\omega_{2}) \alpha(\omega_{2})] d1 d2 d\omega_{1} d\omega_{2}$$
(1.20)

$$|\Psi(1,2)|^2 = \frac{1}{2} \left[|\phi_1(1)|^2 |\phi_1(2)|^2 + |\phi_1(1)|^2 |\phi_1(2)|^2 \right]$$
(1.21)

1.2.1 Two-Electron Integrals

As stated before, the main difficulty of performing calculations on many electron systems is figuring out how to deal with the interactions between the electrons. We can get around this by making the assumption that these interactions can be approximated by figuring out how a single electron interacts with the *average* field generated by all the other electrons. This is called the mean-field method[15]. With this, we can replace the Hamiltonian operator with the one-electron Fock operator which is given below[14]

$$\hat{f}(i) = -\frac{1}{2}\nabla_i^2 - \sum_A \frac{Z_A}{r_{iA}} + v^{HF}(i)$$
(1.22)

The first two terms are combined into an operator called the H^{core} operator $(\hat{h}(i))$ and $v^{HF}(i)$ is the potential generated by all the electrons except the i^{th} one. $v^{HF}(i)$ is composed of two different operators: the Coulomb operator and the exchange operator. The Coulomb operator is intuitive, it is simply the interaction electron 1 experiences when in a Coulomb potential generated by electron 2

$$\hat{J}_b(1)\psi_a(1) = \left[\int \psi_b^*(2)\frac{1}{r_{12}}\psi_b(2)d\mathbf{x}_2\right]\psi_a(1)$$
(1.23)

where $J_b(1)$ is the Coulomb operator for electron 1 when interacting with an electron in spin orbital b and \mathbf{x}_i is the spatial coordinates of electron i. The exchange operator is slightly more complicated than the Coulomb operator. While the Coulomb operator can be defined without a function to operate on (simply remove $\psi_a(1)$ from both sides of Equation 1.23 and it is still a valid operator), the exchange operator only is defined when operating on a function. Its form is given below.

$$\hat{K}_b(1)\psi_a(1) = \left[\int \psi_b^*(2)\frac{1}{r_{12}}\psi_a(2)d\mathbf{x}_2\right]\psi_b(1)$$
(1.24)

where $K_b(1)$ is the exchange operator for electron 1 operating on spin orbital a. At first glance, it might appear to be almost the same as Equation 1.23, but notice that ψ_a has been swapped (or exchanged) with ψ_b inside the integral. The term itself does not really have a classical interpretation, but its need arises due to the use of an antisymmetric wavefunction.

Now it would be helpful to introduce some new notation. The expectation values for these operators are defined as follows

$$\left\langle \psi_a(1) | \hat{J}_b(1) | \psi_a(1) \right\rangle = \int \int \psi_a^*(1) \psi_a(1) \frac{1}{r_{12}} \psi_b^*(2) \psi_b(2) d\mathbf{x}_1 d\mathbf{x}_2 = (aa|bb)$$
(1.25)

$$\left\langle \psi_a(1) | \hat{K}_b(1) | \psi_a(1) \right\rangle = \int \int \psi_a^*(1) \psi_b(1) \frac{1}{r_{12}} \psi_b^*(2) \psi_a(2) d\mathbf{x}_1 d\mathbf{x}_2 = (ab|ba)$$
(1.26)

These are called the two-electron integrals. The Hartree-Fock equation can be written as

$$\left[\hat{h}(1) + \sum_{b \neq a}^{n} \left(J_{b}(1) - K_{b}(1)\right)\right] \psi_{a}(1) = \epsilon_{a} \psi_{a}(1)$$
(1.27)

$$\left\langle \psi_a(1)|\hat{h}(1)|\psi_a(1)\right\rangle + \sum_{b\neq a}^n \left[(aa|bb) - (ab|ba)\right] = \epsilon_a \tag{1.28}$$

where n is the number of spin orbitals in the system and ϵ_a is the energy of an electron in spin orbital a. If instead we are interested in the energy of an entire atom or molecule, the equation becomes

$$\sum_{a}^{n} \left\langle \psi_{a}(1) | \hat{h}(1) | \psi_{a}(1) \right\rangle + \frac{1}{2} \sum_{a}^{n} \sum_{b}^{n} \left[(aa|bb) - (ab|ba) \right] = \epsilon$$
(1.29)

where the factor of one half is multiplied to the two electron terms as a result of the interactions being doubly counted by the summations.

1.2.2 Basis Sets

Back in section 1.2, it was said that there were some ground rules for our wavefunction. The second of these ground rules is that our trial wavefunction (Φ) must meet the boundary conditions for the original problem. Up until now, we have used only spin orbitals (ψ) to describe the wavefunction, which as you'll recall is composed of a spin function, which we have already talked about at length, and a spatial orbital (ϕ) which we have almost completely ignored. I'll discuss the spatial orbitals next.

As mentioned, the overall wavefunction of a system (Ψ) cannot be known exactly unless we are looking only at hydrogen-like atoms. So instead we write the wavefunction as a Slater determinant composed of spin orbitals. What exactly is the mathematical form of these spin orbitals? As it turns out, unless we are talking only about atoms, we have no idea what these are either, even from a numerical stand point. However, we can make a fairly educated guess about what they *should* resemble. The general idea is this: by pre-calculating a set of functions with adjustable parameters (ζ), we can represent a wavefunction with a linear combination of $\Phi(\zeta)$ that adequately reproduces results of numerical calculations of ϕ . Mathematically, this is expressed as[14]

$$\phi_u \approx \sum_{i=1}^K C_{u,i} \Phi(\zeta_{u,i}) \tag{1.30}$$

where $\zeta_{u,i}$ is the i^{th} adjustable parameters of the basis function Φ which is approximating the u^{th} orbital, $C_{u,i}$ is the i^{th} coefficient of i^{th} basis function of the $u^{th} \phi$, and K is the total number of basis functions that make up the basis set. $C_{u,i}^2$ can be thought of as the "weight" of ϕ that $\Phi(\zeta_{u,i})$ makes up.

When choosing the Φ s, our ground rule comes into play. We must choose a function that meets the boundary conditions of the problem, which means that is must go to zero at infinity. Because an atom (or molecule) consists of electrons in the potential generated by one (or many) nuclei, it is reasonable to conclude that the wavefunction would be similar to that of the hydrogen atom. We might initially think to use the exact hydrogen atom solution, but it quickly requires lots of floating point operations to compute which makes it impractical to use for large scale calculations. A more reasonable function is the Slater-type orbital (STO)[16]. These use a different radial function, but still use the same spherical harmonics as the hydrogen-atom like wavefunctions. The radial part of the 1s orbital centered at R_A is shown below

$$\Phi_{1s}^{STO}(r - R_A) = \sqrt{\frac{\zeta^3}{\pi}} e^{-\zeta |r - R_A|}$$
(1.31)

The radial equation for any value of n is

$$\Phi^{STO}(r - R_A) = Nr^{n-1}e^{-\zeta|r - R_A|}$$
(1.32)

where N is a normalization constant. This is a simpler equation to work with than the exact hydrogen atom solution because it does not need to use the Laguerre polynomials. But even with these, problems arise when we try to use them in the two-electron integrals. Because we may be trying to do a two-electron integral over functions which could be located at up to four different centers, we end up with something that is very hard to compute. Therefore, Gaussian-type orbitals (GTOs) have become the preferred functions for producing basis sets. The radial part of a 1s GTO centered at R_A is shown below[17]

$$\Phi_{1s}^{GTO}(r - R_A) = \left(\frac{2\zeta}{\pi}\right)^{\frac{3}{4}} e^{-\zeta |r - R_A|^2}$$
(1.33)

Because the product of two different Gaussians centered at two different locations is a third Gaussian centered at a third location, this makes the two-electron integrals much easier to deal with. The trade off is that GTOs do not as accurately match the hydrogen atom solution as STOs, but this can be fixed somewhat by just using more of them.

All of this reduces our wavefunction issue to a simple optimization problem, which will be discussed more in-depth in Chapter 3.

1.2.3 Hartree-Fock SCF

In the previous sections, we discussed the calculation of the two-electron integrals and introduced the concept of using basis sets to approximate a wavefunction. Now we will discuss how they are actually used. Inspection of the Hartree-Fock operators, Equations 1.23 and 1.24, shows that they depend on the solutions of the Hartree-Fock equations. Consequently, these equations are solved using a technique called the self-consistent field (SCF) method.

SCF method begins with the formation of the density matrices. If we are looking at a single atom, we can exploit the symmetry of the problem by having a smaller density matrix for each orbital symmetry (λ), instead of one large one for the whole system. There are also two types of density matrices, one for contributions from closed shell spinors ($\mathbf{D}_{\mathbf{C}}$) and one for contributions from open shelled spinors ($\mathbf{D}_{\mathbf{O}}$).

Using a procedure developed independently by Roothaan and Hall[15, 18], we first need to find the matrix \mathbf{C} which satisfies

$$\mathbf{FC} = \epsilon \mathbf{SC} \tag{1.34}$$

where **F** is the Fock matrix, ϵ is the vector of eigenvalues, and **S** is the overlap matrix. The matrix elements of **S** are

$$\mathbf{S}_{p_{\lambda},q_{\lambda}} = \langle p_{\lambda} | q_{\lambda} \rangle \tag{1.35}$$

and the non-relativistic **F** for closed shells of symmetry λ is given by

$$\mathbf{F}_{p_{\lambda},q_{\lambda}} = \langle p_{\lambda} | \hat{h}(1) | q_{\lambda} \rangle + \sum_{\mu=1}^{nsym} \sum_{r=1}^{K} \sum_{s=1}^{K} \left(2 \sum_{a=1}^{occ} \mathbf{C}_{r_{\mu},a} \mathbf{C}_{s_{\mu},a}^{*} \right) \left[(p_{\lambda}q_{\lambda} | r_{\mu}s_{\mu}) - \frac{1}{2} \left(p_{\lambda}q_{\lambda} | s_{\lambda}r_{\lambda} \right) \right]$$
(1.36)

where p, q, r, and s are basis functions, K is the total number of basis functions for symmetry μ , and *occ* is the number of occupied closed shells in symmetry μ . Because p and q will always be of the same symmetry, and likewise with r and s, the λ and μ subscripts will be dropped from these indices and instead will be obtained from context. As we can see, \mathbf{F} is itself a function of \mathbf{C} and we are left with a rather disappointing outcome, that in order to find \mathbf{C} , we first must know what it is. And so it would seem that all is lost and all of this hard work was for nothing. And yet, there is a glimmer of hope. \mathbf{F} is made up of two terms, and as only the term corresponding to contributions from the two-electron integrals depends on \mathbf{C} , the term from one-electron integrals can be used independently of \mathbf{C} . Thus, we begin by assuming that \mathbf{F} depends solely on the one-electron term, effectively assuming that $\mathbf{C} = \mathbf{0}$. Solving Equation 1.34 with the H^{core} hamiltonian matrix only will give us the initial guess of \mathbf{C} . With this, we can then resolve \mathbf{F} with the guess of \mathbf{C} and diagonalize the new \mathbf{F} matrix to get another set of values for \mathbf{C} . We can then repeat this process over and over until \mathbf{C} is no longer changing outside an acceptable tolerance at which point we say the calculation has converged. We have now just completed a Hartree-Fock calculation.

1.3 Special Relativity

Another field of physics that was being developed at the same time as quantum mechanics was special relativity (general relativity which involves gravity's effect on spacetime is far, *far* outside the scope of this thesis. I will therefore be referring to special relativity as just relativity from now on). Relativity traces its roots to Michelson and Morley[19] who made the startling observation that all observers, regardless of their frame of reference, will always agree on the speed of light. But it would not be until everyone's favourite Swiss patent clerk decided to examine this issue that the truly profound implications of this observation would be known.

This is perhaps a bit of an aside, but it is simply too interesting to pass up. Consider this thought experiment: you and I are in two different spaceships in space. We will define your frame of reference such that you are stationary at the origin, and that I am flying past you at a constant speed that is arbitrarily close to the speed of light, we will call this speed v. In my spaceship, there is a laser that I have pointed perfectly perpendicular to the direction I am traveling. From my frame of reference, where I am stationary, I turn the laser on and observe photons that move from the laser to the side of my spaceship, a distance equal to d_1 , in time equal to t at the speed of light c. Back in your frame of reference, you are also watching my experiment, but you make some different observations. In the time it take for the photons to move across my spaceship, I move a small distance d_2 . So the total distance you see the photons move is not d_1 , but d_3 which is the hypotenuse of the right angle triangle formed by d_1 , d_2 , and d_3 . But, we both agree that the photons were moving at speed c! So we can not agree on the time it took to do so because $d_3 > d_1$. So you will observe the time it takes for the photons to move to be a time equal to t'. We can derive the relationship between t and t' in the following way.

$$d_1 = ct \qquad \qquad d_2 = vt' \qquad \qquad d_3 = ct' \qquad (1.37)$$

$$d_3^2 = d_1^2 + d_2^2 \tag{1.38}$$

$$(ct')^2 = (vt')^2 + (ct)^2$$
(1.39)

$$(ct)^{2} = (ct')^{2} - (vt')^{2}$$
(1.40)

$$t = t' \sqrt{1 - \frac{v^2}{c^2}} \tag{1.41}$$

Not only does this give the absolutely remarkable result that time is relative, Equation 1.41 also implies that an object can have a maximum speed. But how could this be possible, if I turned on the engine of my spaceship, what's to stop me from just getting faster and faster? The answer is that the mass of an object increases the closer to the speed of light it is. This can be described by [20]

$$m(v) = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \tag{1.42}$$

where m(v) is the mass of an object moving at speed v and m_0 is the rest mass of the object. With this we can see how it would be impossible for an object with mass to move at the speed of light. Its mass would go to infinity and would therefore need an infinite amount of energy to get there.

If we expand Equation 1.42 as a Taylor series centered at zero, we obtain the following equation

$$m(v) = m_0 \left[1 + \frac{1}{2} \frac{v^2}{c^2} + \frac{3}{8} \frac{v^4}{c^4} + \frac{5}{16} \frac{v^6}{c^6} + \frac{35}{128} \frac{v^8}{c^8} + \dots \right]$$
(1.43)

which after rearranging, and multiplying both sides by c^2 gives

$$(m(v) - m_0)c^2 = \frac{m_0v^2}{2} + m_0 \left[\frac{3}{8}\frac{v^4}{c^2} + \frac{5}{16}\frac{v^6}{c^4} + \frac{35}{128}\frac{v^8}{c^6} + \dots\right]$$
(1.44)

So if we take the mass of an object at speed v and subtract the mass of the object and then multiply the result by c^2 , we get the kinetic energy of the object (plus some terms that very quickly go to zero). This is what led Einstein to believe that the total kinetic energy of an object was stored in its mass. He would use this to produce the world's most famous equation

$$E_{kin} = m(v)c^2 \tag{1.45}$$

1.3.1 Relativistic Quantum Mechanics

It would seem that relativity concerns the physics of the very large and fast, while quantum mechanics is concerned with the very small. To merge the two, let us start from the beginning with the time-dependent one-dimensional Schrödinger equation which we will rewrite here in a more general and explicit form[6]

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + \hat{V}(x)\Psi(x,t)$$
(1.46)

where $i\hbar\frac{\partial}{\partial t}$ is the energy operator, $-\hbar^2\frac{\partial^2}{\partial x^2}$ is the momentum squared operator $(\hat{p} = -i\hbar\frac{\partial}{\partial x})$, \hbar is the reduced Planck's constant $(\hbar = \frac{\hbar}{2\pi})$ and $\hat{V}(x)$ is the potential energy operator that the particle described by $\Psi(x,t)$ experiences. The reason we can not use the Schrödinger equation directly in relativistic quantum mechanics is because it treats time and space differently (it depends on only the first derivative of time, but the second derivative of space). In order to fix this, we may express Equation 1.45 in terms of \hat{p} and get[20]

$$E_{kin}^2 = \hat{p}^2 c^2 + m_0^2 c^4 \tag{1.47}$$

If we want to solve this equation for a free particle $(\hat{V}(x) = 0)$, we could put the energy and momentum operator from Equation 1.46 into Equation 1.47 and multiply both sides from the right to obtain

$$-\hbar^2 \frac{\partial^2 \Psi(x,t)}{\partial t^2} = c^2 \left(-\hbar^2 \frac{\partial^2 \Psi(x,t)}{\partial x^2} + m_0^2 c^2 \Psi(x,t) \right)$$
(1.48)

which is called the Klein-Gordon[21, 22] equation for a free particle. We could also solve for a particle of charge q in a electromagnetic field described by potentials \hat{A} and $\hat{\varphi}$ as

$$\left(i\hbar\frac{\partial}{\partial t} - q\hat{\varphi}\right)^2 \Psi(x,t) = c^2 \left[\left(-i\hbar\frac{\partial}{\partial x} - \frac{q}{c}\hat{A}\right)^2 + m_0^2 c^2 \right] \Psi(x,t)$$
(1.49)

Here we are treating time and space exactly the same, but there is a problem. While this equation works perfectly well for spinless particles, we can not ad hoc add spin to this equation like we did with the original Schrödinger equation without violating its Lorentz invariance, which is also important for relativistic theories. Also, because this equation solves for the *square* of the energy, it implies that the energy could both be positive or negative. This is a puzzling result that we will return to later, but for now let us examine how Dirac fixed the issue of introducing spin.

1.3.2 Dirac Equation

Dirac^[23] began with the Klein-Gordon equation which may be written in a three-dimensional form as

$$\boldsymbol{\pi}_{0}^{2} - \left[\sum_{u=x,y,z} \boldsymbol{\pi}_{u}^{2} + m_{0}^{2} c^{2}\right] = 0$$
(1.50)

$$\boldsymbol{\pi}_{0} = \frac{i\hbar\frac{\partial}{\partial t} - q\hat{\varphi}}{c}, \quad \boldsymbol{\pi}_{u} = -i\hbar\frac{\partial}{\partial u} - \frac{q}{c}\hat{A}$$
(1.51)

Dirac wanted to write this equation as the product of one equation and its conjugate, which can be done as follows

$$\left(\boldsymbol{\pi}_{0} + \left[\sum_{u=x,y,z} \alpha_{u} \boldsymbol{\pi}_{u} + \alpha_{0} m_{0} c\right]\right) \left(\boldsymbol{\pi}_{0} - \left[\sum_{u=x,y,z} \alpha_{u} \boldsymbol{\pi}_{u} - \alpha_{0} m_{0} c\right]\right) = 0 \quad (1.52)$$

so long as we restrict α as

$$\alpha_i^2 = 1, \quad \alpha_i \alpha_j + \alpha_j \alpha_i = 0 \quad \text{for} \quad i \neq j$$
 (1.53)

It's clear that the α s must be matrices. The simplest of these that meet the requirements of Equation 1.53 are

$$\alpha_i = \begin{pmatrix} \mathbf{0} & \sigma_i \\ \sigma_i & \mathbf{0} \end{pmatrix} \quad \text{for} \quad i \neq 0 \tag{1.54}$$

$$\alpha_0 \equiv \beta = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \tag{1.55}$$

where σ_i are the Pauli spin matrices for $i = x, y, z, \mathbf{0}$ is a 2 × 2 matrix of zeros, and **I** is a 2 × 2 identity matrix[20]. We now have two different operator equations

$$\left(\boldsymbol{\pi}_{0} + \sum_{u=x,y,z} \alpha_{u} \boldsymbol{\pi}_{u} + \beta m_{0} c\right) \Psi(x,y,z,t) = 0$$
(1.56)

$$\left(\boldsymbol{\pi}_{0} - \sum_{u=x,y,z} \alpha_{u} \boldsymbol{\pi}_{u} - \beta m_{0} c\right) \Psi(x,y,z,t) = 0$$
(1.57)

Equation 1.56 will give negative energy and Equation 1.57 will give positive energy. The positive energy solutions correspond to electrons. The negative energy solutions correspond to antimatter, which is remarkable because antimatter would not be discovered until years later[24]. The stationary states (time-independent) for the electron then become

$$\left(E - V - \beta m_0 c^2 - c \sum_{u=x,y,z} \alpha_u \boldsymbol{\pi}_u\right) \Psi(x,y,z) = 0$$
(1.58)

where $V = q\hat{\varphi}$. Introducing α as a 4×4 matrix means that Ψ must also have four components. It is typically written as

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} \psi \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ \phi \end{pmatrix} = \begin{pmatrix} \psi \\ \phi \end{pmatrix}$$
(1.59)

where $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$ are called spinors. $\boldsymbol{\psi}$ is called the large component and $\boldsymbol{\phi}$ is the small component.

1.3.3 Kinetic Balancing

Recall that Equation 1.58 is only half of the total equation. We still have all of the negative energy solutions to deal with. If we were to try an use Equation 1.58 as is, the numerical methods we use of solving it would find these negative energies, and as there is no lower bound on the negative solutions, our solutions to the equation would all drop to negative infinity. We can solve this problem if we assume that all the infinite number of negative energy states are filled with an infinite number of positrons. This means that the electron can not drop into the negative energies due to the Pauli exclusion principle. Mathematically, we can reproduce this idea using a procedure called kinetic balancing, which is done in the following way[20].

Using the spinors, we can write Equation 1.58 as a matrix multiplication problem of the form

$$\begin{pmatrix} (V+\beta m_0 c^2) & c(\boldsymbol{\sigma}\boldsymbol{\pi}) \\ c(\boldsymbol{\sigma}\boldsymbol{\pi}) & (V+\beta m_0 c^2) \end{pmatrix} \begin{pmatrix} \boldsymbol{\psi} \\ \boldsymbol{\phi} \end{pmatrix} = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \begin{pmatrix} \boldsymbol{\psi} \\ \boldsymbol{\phi} \end{pmatrix}$$
(1.60)

where $\sigma \pi = \sum_{u=x,y,z} \alpha_u \pi_u$. This is equivalent to adding the following two equations together

$$(E - V - m_0 c^2)\boldsymbol{\psi} - c(\boldsymbol{\sigma}\boldsymbol{\pi})\boldsymbol{\phi} = 0$$
(1.61)

$$(E - V + m_0 c^2)\boldsymbol{\phi} - c(\boldsymbol{\sigma}\boldsymbol{\pi})\boldsymbol{\psi} = 0$$
(1.62)

We can set where the energy is zero to anywhere we want, so let us make zero the energy of a free electron at rest ($\epsilon = E - m_0 c^2$). Equations 1.61 and 1.62 now become

$$(\epsilon - V)\boldsymbol{\psi} - c(\boldsymbol{\sigma}\boldsymbol{\pi})\boldsymbol{\phi} = 0 \tag{1.63}$$

$$(\epsilon - V + 2m_0c^2)\boldsymbol{\phi} - c(\boldsymbol{\sigma}\boldsymbol{\pi})\boldsymbol{\psi} = 0$$
(1.64)

We can rewrite Equation 1.64 as

$$\boldsymbol{\phi} = \left(1 + \frac{(\epsilon - V)}{2m_0 c^2}\right)^{-1} \frac{1}{2m_0 c^2} \boldsymbol{\sigma} \boldsymbol{\pi} \boldsymbol{\psi}$$
(1.65)

To a good approximation, $\epsilon - V$ will be much smaller than $2m_0c^2$, so we can assume the term in parentheses is equal to 1. Therefore, the small component can be written in terms of just ψ and becomes

$$\boldsymbol{\phi} = \frac{\boldsymbol{\sigma}\boldsymbol{\pi}}{2m_0c^2}\boldsymbol{\psi} \tag{1.66}$$

Not only does this make solving the Dirac equation much simpler (we only need to solve for ψ instead of ψ and ϕ) it also "hides" the negative energies from numerical methods. Note, though, that it relies on the assumption that $\epsilon - V$ is much smaller than $2m_0c^2$. If this is not the case, such as in the electrons in the heaviest known elements, then this procedure will fail and we will get energies that are lower than they should be. When this occurs, we say that there is variational prolapse of the wavefunction.

1.3.4 The Dirac Hydrogen-Like Atom

Up until now, we have only looked at what Dirac's theory says about a free electron (well, a "free" electron in the presence of an infinite amount of positrons). In the case of hydrogenlike atom solutions, the quantum numbers are similar to the non-relativistic theory. They are: the principal quantum number (n = 1, 2, 3, ...), the azimuthal quantum number (l = 0, 1, 2, ..., n - 1), the angular momentum quantum number $(j = |l \pm \frac{1}{2}|)$, and the magnetic quantum number (m = -j, -j+1, ..., j-1, j). The energy in terms of the quantum numbers is given by [20]

$$E_{n,j} = -\frac{1}{2n^2} \left[1 + \frac{1}{nc^2} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) \right]$$
(1.67)

It can be seen that there is a splitting in the energy levels of spinors with the same azimuthal number, whereas in the non-relativistic theory, orbitals with the same azimuthal number would all be perfectly degenerate.

1.3.5 Relativistic Effects

The effects of relativity have a dramatic effect on chemistry. Two classic examples are gold's distinctive colour, and mercury being the only metal that is liquid at room temperature. In the case of gold, its $6s_{1/2}$ electrons are lowered in energy and its $5d_{5/2}$ electrons are raised. This shifts its absorption region into the blue end of the spectrum, making it appear yellow[25]. The $6s_{1/2}$ electrons of mercury are similarly stabilized and since its $5d_{3/2}$ and $5d_{5/2}$ orbitals are filled, it behaves quite like a noble gas, making bonding quite difficult at room temperature[26].

Relativistic effects are broken up into two categories: primary and secondary effects. Primary effects are due to the contraction of the s and p electrons. The non-relativistic Bohr radius for the 1s electron of hydrogen is[8]

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_0e^2} \tag{1.68}$$

where ϵ_0 is the permittivity of free space, \hbar is the reduced planks constant, e is the charge of an electron, and m_0 is the mass of an electron at rest. Recall from Equation 1.42 that the mass of an object increases with its speed. If we substitute m(v) from Equation 1.42 for m_0 into Equation 1.68 we get

$$a_v = \frac{4\pi\epsilon_0 \hbar^2 \sqrt{1 - \frac{v^2}{c^2}}}{m_0 e^2}$$
(1.69)

Dividing Equation 1.69 by 1.68 gives

$$\frac{a_v}{a_0} = \sqrt{1 - \frac{v^2}{c^2}} \tag{1.70}$$

which is less than 1 and will get closer and closer to zero as v increases (v will increase in proportion to the nuclear charge). This contraction stabilizes the electrons, making them more inert.

Secondary effects are a direct result of the electron density contraction. The contraction of these electrons leads to greater shielding of the nucleus, reducing its effective nuclear charge. This causes the d and f electrons to feel a smaller attraction to their nucleus, which makes their orbitals enlarge. This destabilizes these electrons, making them more reactive[20].

1.3.6 Gaussian Nucleus

Up till now, we have assumed the nucleus can be represented as a point. For many applications this works just fine, but it can make it difficult to find convergence when relativity is considered. Therefore, it is helpful to use a model more grounded in reality in this case. One such model is the Gaussian nucleus. This changes the potential in Equation 1.60 to

$$V(\mathbf{r}) = Z\left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \int \frac{e^{-\alpha(\mathbf{r}-\mathbf{R})^2}}{|\mathbf{r}-\mathbf{R}|} d\mathbf{R}$$
(1.71)

where \mathbf{r} is the coordinates of an electron, \mathbf{R} is the coordinates of the nuclei, Z is the nuclear charge, and α is an estimation of the "size" of the nucleus. This is usually approximated using the root-mean-square (RMS) radius of the nuclei[27], which can be related to the mass of the nucleus by[28]

$$\sqrt{\langle R^2 \rangle} = \left(0.836 A^{1/3} + 0.570 \right) \tag{1.72}$$

where $\langle R^2 \rangle$ is the mean-square radius in femtometers, and A is the mass of the nucleus. Converting the RMS into atomic units and substituting its value into the following equation gives the value of $\alpha[27]$

$$\alpha = \frac{3}{2\left\langle R^2 \right\rangle} \tag{1.73}$$

Chapter 2 cudaDFRATOM

2.1 Introduction

In this Chapter, I present a program that can optimize four-component relativistic basis sets. It was adapted from Matsuoka's and Watanabe's DFRATOM program[29]. My program was written in the CUDA Fortran programming language[30], and so I have called it cudaDFRATOM. In the following sections I give an introduction to programing with CUDA Fortran, and then I give a detailed explanation of the algorithms cudaDFRATOM uses. Finally, I show how my new program is able to outperform the original.

2.2 GPU Architecture

While general purpose computing on graphics processing units (GPGPU) (GPUs) has been adopted by the high performance computing (HPC) community for quite some time, it can seem quite complex to the uninitiated. While most quantum chemists who decide to dip their toes into computational waters can get away with having little to no understanding of what is actually going on under the hood when programming for a central processing unit (CPU), the same can not at all be said for GPUs. Therefore, in this section I will explain how a GPU works in order to help understand the terms and techniques used in the following chapter. As cudaDFRATOM was optimized for the NVIDIA Tesla C2050, I will be referring to the Tesla C2050 specifications for examples when needed. I will begin with the most granularity possible, and zoom out so that by the end of this section, the reader should come away prepared for the rest of this chapter. The bulk of this section has been adapted from [31, 30] and is based on my own experience.

2.2.1 Threads, Blocks, and Grids

The most granular element of computation on a GPU is the thread. When a CUDA function or subroutine (hereafter called a kernel) is called, it is a thread that actually executes the code. What makes GPGPU so powerful is that while a thread in a kernel is always executing the same code, the data a thread works with can be completely different between threads. This method of parallelism is called single instruction, multiple data (SIMD).

32 threads are organized into a structure called a warp. Within a warp, all threads execute code in lock-step. If a condition arises where some threads in warp must execute some code, and other threads in the same warp execute some other code (for instance in an **if else** statement), this leads to serialization of code execution, a process called warp divergence. In a worst-case scenario, this could cause all 32 threads to execute serially which could lead to a massive hit to performance.

Warp divergence can also cause warps to fall behind other warps and has the potential to cause race conditions to appear. A race condition appears when different threads need to use the same memory location, but there is nothing in the code to enforce the order the threads will access the memory location. If one warp needs to read data written by another warp that is several steps behind, this can cause all kinds of confusing errors to appear. Therefore, it is generally advisable to avoid warp divergence whenever possible. But, for programs of any considerable usefulness, warp divergence will be inevitable. Thankfully, NVIDIA has included the **syncthreads** command which provides a barrier that all threads within a block must meet before any can continue.

The next highest structure is the thread block, or block for short. Simply put, a block is a collection of one or more threads. When a kernel is called, the block scheduler assigns each block to a streaming multiprocessor (SM). How many blocks a SM can run at once depends on the resources each block uses (more on this in section 2.2.2), but no more than 8 blocks per SM can ever be run at once on the C2050. Blocks also add an element of dimensionality to threads through the thread index (*threadIdx*) variable. This variable has three parts, *threadIdx.x*, *threadIdx.y*, and *threadIdx.z*¹. These variables make dealing with matrixes and arrays much simpler and can help with parallelizing large nested loops. The size of dimensions of the grid can be accessed through the *blockDim* variable. *blockDim* also has x, y, and z parts. These variables are all integer type, and the *threadIdx* variables range from 1 in Fortran (or 0 in C/++) to the relevant part of *blockDim* in Fortran (or *blockDim* -1 in C/++). The *threadIdx* set of variables are all reset at the boundary of each block.

Finally there is the grid. The grid is the entire collection of blocks that are launched for

¹Note that in Fortran, the x, (or y or z) part of the *threadIdx* variable would be written as *threadIdx*%x. I find the C style dot notation to be more visually appealing, so that is what is used in this thesis.

a kernel. The grid gives a dimensionality to blocks through the blockIdx variable which has similar parts to the threadIdx variable. The grid also has the gridDim variable which is analogous to blockDim.

2.2.2 Memory

To simplify the discussion of the kinds of memory available on a GPU we will limit ourselves to the three main types. They are the global memory, the shared memory, and the register memory. Because the execution time of a calculation is often not limited by the actual number of floating point operations to perform, but rather the reading and writing to memory, it is essential to be sure that the three main types of memory are managed correctly.

Global memory is both the most plentiful and the slowest available memory on a GPU. In a typical calculation, global memory will be allocated in code executed by the CPU (host). Data will be uploaded to the allocated memory and then used by the GPU (device). Global memory is distinct from the other kinds of device memory in that it can be read from and written to by all threads currently executing. This can allow threads of one block to pass messages to threads in an other block, but great care must be taken to avoid race conditions. There is an additional caveat with global memory in that if threads are reading from noncontiguous memory locations, then memory bandwidth plummets. There is also a problem when multiple threads try to read from the same location. Instead of being one transaction, the read is serialized which leads to a massive performance penalty. It is therefore to the programmers advantage to write their kernels with as little use of the global memory as possible.

Shared memory, as its name implies, is shared and private to threads in a single block. It can be accessed much faster than global memory, but this comes at the cost of a much reduced volume. The amount of it available per SM varies with hardware generation, but the maximum available on our card is 48KB. This amount is shared among all blocks that are running on the SM, so the amount available per block will typically be even less. Also, there is no guarantee that memory loaded by one thread will be available to all other threads right away, only a call to **syncthreads** ensures proper loading. But, when used properly, shared memory is indispensable for speeding up calculations. It does not suffer from threads in a warp read from the same memory location a "broadcast" occurs. This means that instead of the read being serialized, all threads are able to read the data in one transaction. Shared memory is also distinct from global memory in that instead of being declared in the device code. This is done by giving the variable the "shared" attribute in its declaration. However, one must be careful not to overuse the shared memory.

As mentioned, there is only 48KB available per SM. If a block needs more than is available, the function will fail to execute. It can also affect the occupancy of the kernel, a concept that will be explained later on.

Lastly there is the register memory. This is the fastest memory available and is also private to an individual thread. Figure 2.1 shows the hierarchy of the grid, blocks, and threads, as well as how each memory type is localized. On the Tesla C2050, there are a total of 32768 32-bit registers available per SM. An individual thread in a block can use no more than 63 registers, and if the number of threads in a block times the number of registers needed per thread for a kernel is larger than the total registers available per SM then the execution of the kernel will fail. If a thread needs more memory than the registers will allow, then "register-spilling" takes place. This means that instead of a variable being stored into a register, it "spills over" into a fourth memory type called local memory. Local memory is really just a section of the global memory and comes with all the problems that global memory has, but the compiler is able to arrange it such that it can be read efficiently without the programmer having to worry about this. There is no way for a programmer to specify which variables will be stored in register or local memory, the compiler handles all of this. There are compiler flags which can change the maximum amount of registers per thread allowed which will prompt the compiler to place more data into local memory. While this may sound like a bad idea, we will see in the next section how there are situations where this might be useful.

2.2.3 Occupancy and Performance

Having described the various resources, we can talk about how they can be used most effectively. The occupancy of a kernel is the number of warps that are actually able to run on a SM divided by the maximum possible warps an SM can run. Occupancy is important, as it determines the maximum number of blocks, and thus threads that are able to run simultaneously. The occupancy of a kernel is determined by three factors: the block size, the amount of shared memory per block, and the number of registers used per thread. While block size and shared memory are explicitly set by the programmer, it is next to impossible to guess how registers will be used before compile time. Thankfully, there are compiler flags that will display this information.

Armed with the resources our kernel will need, we can now determine its occupancy. The "CUDA Occupancy Calculator" is an Excel spreadsheet provided by NVIDIA and is an indispensable tool. We can input the needed resources and the hardware generation of our card and then receive the occupancy of the current resource configuration, where the bottleneck of the current configuration is, as well as information on how the occupancy will



Figure 2.1: Architecture of a GPU. Organization of threads and blocks in the grid, and the location of different memory types within them. The grid is coloured dark blue, blocks are coloured light blue, and threads are coloured cyan. The global memory is coloured red, shared memory is coloured orange, and register memory is coloured yellow. The numbers in parenthesis indicate the block or thread's block Idx or thread Idx variables. In this particular case, block Dim = (8, 4) and grid Dim = (2, 2). A thread is able to access memory that is inside its registers, but not the registers of other threads, and memory that is inside the shared memory of its block, but not the shared memory of other blocks. All threads can access all of the global memory.

change upon tweaking the configuration. In some sense, the best block size is determined by how the other resources are used. Therefore, in order to maximize the occupancy, we must first make sure that we are correctly using the memory provided.

Registers are the fastest memory available, but they are also the easiest to overuse. Therefore, they are best suited for small variables that need to be referenced frequently, such as accumulators. Shared memory is best used for storing large sections of non-contiguous data stored in the global memory. Finally, data that is able to be stored such that it can be accessed effectively, or is infrequently used, might best be left in the global memory.

As with everything, these rules are only guidelines. The best resource configuration will be individual not only to every kernel, but also to the GPU it is to be run on. The best way to maximize the efficiency of a calculation is to make minor alterations to where data is stored and play around with the code. Finally, it might not always be the best idea to maximize the occupancy of a kernel. If the bottleneck is not the actual calculation, but how fast the data can be read, then it might be advantageous to fill up the registers and shared memory as much as possible and have a very low occupation.

2.2.4 Matrix Multiplication Example

To complete the introduction to CUDA programming, we will go over a real example of CUDA Fortran code. For our example, we will examine code that performs matrix multiplication on matrices of arbitrary dimensions. This makes use of all the concepts we've covered so far, so it will be a good exercise to examine. The code is given below.

```
module mat_mul
    implicit none
    integer, parameter :: dp = kind(0.d0)
    integer, parameter :: block_dim = 16
    integer, constant :: rowA, colA, rowB, colB
    contains
      attributes(global) subroutine mat_mul_kernel(inputA, inputB, output)
        real(dp), dimension(:,:) :: inputA, inputB, output
        real(dp) :: total
        real(dp), shared, dimension(block_dim, block_dim) :: s_tileA, s_tileB
        integer :: x, y, i, j
        x = threadIdx%x + blockDim%x * (blockIdx%x - 1)
13
        y = threadIdx%y + blockDim%y * (blockIdx%y - 1)
14
        total = 0.0_dp
        do i = 0, colA - 1, block_dim
          call syncthreads()
18
          if ((x <= rowA) .and. (threadIdx%y + i <= colA)) then
            s_tileA(threadIdx%x, threadIdx%y) = inputA(x, threadIdx%y + i)
20
```

```
else
21
            s_tileA(threadIdx%x, threadIdx%y) = 0.0_dp
          endif
          if ((threadIdx%x + i <= rowB) .and. (y <= colB)) then</pre>
            s_tileB(threadIdx%x, threadIdx%y) = inputB(threadIdx%x + i, y)
26
          else
            s_tileB(threadIdx%x, threadIdx%y) = 0.0_dp
28
          endif
30
          call syncthreads()
          do j = 1, block_dim
            total = total + s_tileA(threadIdx%x, j) * s_tileB(j, threadIdx%y)
34
          enddo
36
        enddo
37
        if((x <= rowA) .and. (y <= colB)) then
          output(x, y) = total
40
        endif
41
      end subroutine mat_mul_kernel
42
  end module mat_mul
43
44
45 program main
    use cudafor
46
    use mat_mul
47
    implicit none
48
    ! Host variables
49
    real(dp), allocatable, dimension(:, :) :: inputA, inputB, output
50
    ! Device variables
    real(dp), device, allocatable, dimension(:, :) :: d_inputA, d_inputB,
     d_output
    ! For generating random numbers
    integer, allocatable, dimension(:) :: seed
    integer :: n
    ! block and grid dimensions
56
    type(dim3) :: blockDim, gridDim
57
58
    rowA = 1024
59
    colA = 432
    rowB = colA
    colB = 1783
    ! Set up random number generator
64
    call random_seed(size = n)
    allocate(seed(n))
66
```

```
! Set seed to a constant so we always get the same matrices
67
    seed = 150987
69
    call random_seed(put = seed)
    deallocate(seed)
70
71
    ! Allocate host matrices and set up matrices
72
    allocate(inputA(rowA, colA))
73
    allocate(inputB(rowB, colB))
    allocate(output(rowA, colB))
76
    call random_number(inputA)
    call random_number(inputB)
78
    ! Allocate and upload device data
80
    allocate(d_inputA(rowA, colA))
81
    allocate(d_inputB(rowB, colB))
82
    allocate(d_output(rowA, colB))
83
    d_inputA = inputA
84
    d_inputB = inputB
85
86
    blockDim = dim3(block_dim, block_dim, 1)
87
    gridDim = dim3((rowA - 1) / block_dim + 1, (colB - 1) / block_dim + 1, 1)
88
89
    call mat_mul_kernel <<<gridDim, blockDim>>> (d_inputA, d_inputB, d_output)
90
91
    ! Download device data
92
    output = d_output
93
    ! Deallocate variables
    deallocate(d_inputA)
96
    deallocate(d_inputB)
    deallocate(d_output)
    deallocate(inputA)
99
    deallocate(inputB)
    deallocate(output)
  end program main
```

Listing 2.1: Matrix multiplication kernel

Lines 1 - 43 define a module which contains a matrix multiplication kernel. The kernel takes the matrices inputA and inputB, multiplies them, and stores the result in output. The kernel has the attributes(global) attribute, which means that it can be called from either device or host code. rowA, colA, rowB, and colB are the rows and columns of inputA and inputB. Because they are small and don't change over the course of the calculation, they get stored in a special memory type called constant memory. This is a small cache of read only memory that is 64KB in size and allows for constant values to be read very quickly.

There are two shared variables, s_tileA and s_tileB. Each of these are square matrices with dimensions of block_dim and these will be used to store sections or "tiles" of inputA and inputB respectively. We want each thread to do all the calculations needed to compute a simple element of output. Line 13 and 14 use the threadIdx, blockDim, and blockIdx variables so that each thread gets a unique combination of x and y values. x corresponds to a row of the output matrix and y corresponds to a column, so each thread is then uniquely mapped to an element of output. We will see in the host code how these index values are determined, but for now it is sufficient to know that there will be at least as many threads as elements of output.

Lines 17 - 37 are where the actual calculation takes place. For each iteration of the loop, a different tile of inputA and inputB is fetched from the global memory and stored into the shared memory. The reason for using this tiling approach can be seen when we consider how the threads must read inputB. If we did not use shared memory, the loop would just be total = total + inputA(x, i) * inputB(i, y). In this case, access to inputA is coalesced, but access to inputB is not. Therefore, the kernel will be stunted due this unoptimized memory usage. Instead, we load tiles in a coalesced manner into the shared memory, synchronize the threads, and then read through the shared memory in an uncoalesced fashion which carries no penalty. At the end of each loop, the tiles are moved in the y direction for inputA and in the x direction for inputB, and the process repeats. Notice how it is possible that a tile might fall on the boundary of an input matrix. This is why there are checks to make sure the coordinates of the tile don't exceed the boundaries of a matrix so we don't start reading garbage.

In the host code on lines 45 - 102, we have two sets of variables, those for the host and those for the device. Notice how device variables have the device attribute. For clarity, they are given the same name as their host variables but with a d_ prefix. We now assign constant variables from line 5 to arbitrary values. Next we set up the random number generator, allocate the host matrices memory, and randomly initialize the input matrices. Then the device variables are allocated memory and the host data is then uploaded to the GPU. The block and grid dimensions are set up on lines 87 and 88. blockDim and gridDim are variables of type(dim3) which is a tuple that is defined in the cudafor module. The block has two dimensions containing block_dim² threads. The grid also has two dimensions, and as we need one thread per element of output we perform a calculation which returns the minimum number of blocks that will cover it. Finally, we launch the kernel on line 90 using the <<< >>> operators to provide the grid and block dimensions, download the result from the GPU, and deallocate the memory.

2.3 Program flow in cudaDFRATOM

In this section, the control flow of a typical calculation is given.

Step 1. The input file is read by the *intin* subroutine. If needed, the basis set and openshell configurations are calculated by *formbs* and *find_bin_configurations* respectively. The options set in the input file are rewritten to stdout.

Step 2. The calculation of small arrays and other constants is performed by *calc_parameters* and *bsnorm. calc_parameters* calls *bcoef* and *setvc*.

Step 3. The mapping of threads to the unrolled one and two-electron integral matrixes are calculated by *lmpqrsa* on the GPU. All other data from step 1 and 2 is then uploaded to the GPU.

Step 4. The one and two electron integrals are calculated on the GPU by eint1gpu and eint2gpu respectively.

Step 5. The initial guess of the density matrix is calculated by guess on the GPU. This is done by the diagonalization of the one-electron Hamiltonian matrix.

Step 6. scfiter then performs the SCF iterations until convergence of the density matrix has been reached, or the maximum number of iterations has been reached. SCF is performed with cuSOLVER functions, as well as a few custom helper functions. The converged eigenvectors, values, and energies are downloaded from the GPU and then written to stdout.

Step 7 (optional). If jobtyp='bsopt', then an optional basis set optimization is carried out. This starts by assigning pointers to variables on the CPU and GPU through **hookup_cpu** and **hookup_gpu**. Then, the four well-tempered basis set (WTBS) parameters are optimized by **newuoa**. **newuoa** calls **calc_energy** which essentially reconstructs the basis set from new parameters from **newuoa**, then repeats steps 2 - 6 and feeds the energy back into **newuoa**. This repeats until optimal WTBS parameters have been found.

2.4 Alterations of DFRATOM for CUDA

While almost all of the code from the original DFRATOM[29] was modified in some way, the most extreme changes were the integral evaluation and the formation of the P and Q matrixes. Therefore, we will discuss these changes in detail in this section.

2.4.1 Two-electron Integrals

The original DFRATOM calculates the two electron integrals with a long series of nested for loops. Working from the outside in, the indices of the loops are L, P, Q, M, R, and Swhere L and M are spinor symmetries, P and Q are basis functions of symmetry L, and Rand S are basis functions of symmetry M. The pseudocode for these is shown in Algorithm
1 where nsym is the total number of symmetries, and nbs(i) is the number of basis functions for symmetry species *i*. Thus, each set of J and K integrals is uniquely defined by its L, M, P, Q, R, and S values. In order to have an effective CUDA implementation of this algorithm, we need to find a way to map these six numbers to CUDA threads. The simplest approach would be to map the values of L, P, and Q onto the *threadIdx.x*, *threadIdx.y*, and *threadIdx.z* variables for each thread, launch the needed number of blocks, and then have each thread loop over the remaining indices. The pseudocode for this can be seen in Algorithm 2. A similar method is employed by many other programs, and for larger systems it works perfectly well. But because this program is for only single atoms, problems begin to appear.

Al	gorit	hm 1	The	original	
----	-------	------	-----	----------	--

```
for L = 1 to nsym do
  for P = 1 to nbs(L) do
    for Q = 1 to P do
      for M = 1 to L do
        if L = M then
          maxr = P
        else
          maxr = nbs(M)
        end if
        for R = 1 to maxr do
          if (L = M) and (P = R) then
            maxs = Q
          else
            maxs = R
          end if
          for S = 1 to maxs do
            compute the J and K integrals of L, M, P, Q, R, and S
          end for
        end for
      end for
    end for
  end for
end for
```

The first problem arises due to warp divergence: as the maximum values of M, R, and S depend on L, P, and Q, different threads will have a different number of loops to complete than others. Because a streaming multiprocessor (SM) must finish the block it is currently working on before it can grab another, there is the possibility that most of the threads in a block are idling while waiting for others in the same block to finish. The second problem with this method is that there will always be several blocks which have threads that remain

Algorithm 2 Easy code

L = threadIdx.x + (blockIdx.x - 1) * blockDim.xP = threadIdx.y + (blockIdx.y - 1) * blockDim.yQ = threadIdx.z + (blockIdx.z - 1) * blockDim.zif $(L \leq nsym)$ and $(P \leq nbs(L))$ and $(Q \leq P)$ then for M = 1 to L do if L = M then maxr = Pelse maxr = nbs(M)end if for R = 1 to maxr do if (L = M) and (P = R) then maxs = Qelse maxs = Rend if for S = 1 to maxs do compute the J and K integrals of L, M, P, Q, R, and S end for end for end for end if

idle throughout the block's runtime, no matter what. This can be seen more clearly in Figure 2.2. The third problem with this is that with the maximum values for L, P, and Q available for a single atom, there might not even be enough combinations to completely fill the GPU. While all of these issues begin to disappear once the number of integrals to evaluate becomes large enough, we are still very much in the range where they are in play. Therefore a smarter algorithm had to be used.

The second problem can be solved by restricting the dimensionality of the solution instead of the using the three dimensional one of Algorithm 2. We might consider using a two dimensional solution, but then we still will have blocks with idle threads which can be seen in Figure 2.3. By restricting ourselves to only using threadIdx.x, we ensure that only the last block to run will have the possibility of having threads remaining idle throughout the block's runtime as shown in Figure 2.4.

The first and third problems can be solved by having each thread calculate one and only one set of J and K integrals. If we start with a valid combination of L, M, P, Q, R, and S values, we can very easily figure out which thread will calculate that set of integrals by using the following equations:

$$n'(j) = \frac{j^2 + j}{2} \tag{2.1}$$

$$y = n'(nbs(L-1)) + n'(P-1) + Q$$
(2.2)

$$x = n'(nbs(M-1)) + n'(R-1) + S$$
(2.3)

$$i = n'(x) + y \tag{2.4}$$

$$i_{max} = n'(\sum_{j=1}^{nsym} n'(nbs(j)))$$
 (2.5)

where nbs(0) = 0 and i = threadIdx.x + (blockIdx.x - 1) * blockDim.x. Starting with a value of i and working our way back is a much more challenging task. It becomes easier if we reframe it in the following way.



Figure 2.2: Two-electron integral layout: naive implementation. Mapping of integrals to threads using Algorithm 2. The basis set used had nsym = 7 with nbs(i) = (30, 25, 25, 20, 20, 15, 15). The blockDim = (1, 32, 32) and gridDim = (7, 1, 1). Each histogram is one block of threads, where the horizontal axes are the threadIdx.y and threadIdx.z variables, and the vertical axis is the number of Two-Electron Integrals it must compute. Notice that in all blocks there are threads that calculate no integrals and therefore are idle throughout the lifetime of the block. Also note that the number of integrals each thread must calculate grows both from block to block, and from thread to thread within a block. Both of these factors make this algorithm an undesirable choice.



Figure 2.3: Two-electron integral layout: 2D blocks and grid. Orange lines indicate the border of blocks. Notice that many blocks have idle threads.



Figure 2.4: Two-electron integral layout: 1D blocks and grid. Orange lines indicate the border of blocks. Notice that only the last block contains idle threads.

Consider Figures 2.5 and 2.6. Figure 2.5 shows the top half of the symmetric two-electron integral matrix for a problem with nsym = 2 and 3 basis function for symmetry one, and 2 for symmetry two. Figure 2.6 shows the same but mapped onto a vector representation. In each element of both figures there is a set of seven numbers. The top two are L and M, then P and Q, then R and S, and the last number is the value of i for the thread calculating that integral. With this, it can be seen from the matrix representation that each element in the same row have the same M, R, and S values and the elements in the same column have the same L, P, and Q values. Therefore, finding out which column the element belongs to gives us the value for y, and finding the row give us the value of x. This can be done with the binary search algorithm shown in Algorithm 3.

Algorithm 3 Binary search for x and y

```
if theadIdx.x < nsym then
  s_nsym = nsym
  s_nbs(threadIdx.x) = nbs(threadIdx.x)
  s_nprime(threadIdx.x) = n'(s_nbs(threadIdx.x))
end if
call syncthreads
i = threadIdx.x + (blockIdx.x - 1) * blockDim.x
if i \leq i_{max} then
  low = 1
  high = \mathbf{sum}(s\_nprime(1:s\_nsym))
  while low \leq high do
mid = \frac{(low+high)}{2}
    mid = \underbrace{\frac{2}{2}}_{lownum} = \frac{(mid-1)(mid-2)}{2} + mid
     highnum = lownum - 1 + mid
     if (i \leq highnum) and (i \geq lownum) then
       y = mid
       \mathbf{exit}
     else if i > highnum then
       low = mid + 1
     else if i < lownum then
       high = mid - 1
     end if
  end while
  x = i - lownum + 1
end if
```

In this algorithm, variables with the s_{-} prefix refer to those in the shared memory, and lownum and highnum refer to the minimum and values that *i* could have for the current guess (mid) of y. From here, L can be found with Algorithm 4, and P and Q can be found with Algorithm 5. The same set of algorithms can then be used to get M, R, and S

	1 1	1 1	1 1	1 1	2 1	2 1	2 1
1 1 2 1	2 2	3 1	3 2	3 3	1 1	2 1	2 2
1 1 1 1	1 1	1 1	1 1	1 1	1 1	1 1	1 1
1 2	4	7	11	16	22	29	37
1 1	1 1	1 1	1 1	1 1	2 1	2 1	2 1
2 1	2 2	3 1	3 2	3 3	1 1	2 1	2 2
2 1	2 1	2 1	2 1	2 1	2 1	2 1	2 1
3	5	8	12	17	23	30	38
	1 1	1 1	1 1	1 1	2 1	2 1	2 1
	2 2	3 1	3 2	3 3	1 1	2 1	2 2
	2 2	2 2	2 2	2 2	2 2	2 2	2 2
	6	9	13	18	24	31	39
•		1 1	1 1	1 1	2 1	2 1	2 1
		3 1	3 2	3 3	1 1	2 1	2 2
		3 1	3 1	3 1	3 1	3 1	3 1
		10	14	19	25	32	40
			1 1	1 1	2 1	2 1	2 1
			3 2	3 3	1 1	2 1	2 2
			3 2	3 2	3 2	3 2	3 2
			15	20	26	33	41
				1 1	2 1	2 1	2 1
				3 3	1 1	2 1	2 2
				3 3	3 3	3 3	3 3
				21	27	34	42
					2 2	2 2	2 2
					1 1		
					1 1		
					28		
						2 2	
						2 1	2 1
							44
L M							2 2
P Q							2 2
RS							2 2
I							45

Figure 2.5: Two-electron integral matrix as a matrix: The top triangle of the two-electron symmetric matrix in a matrix representation. In this instance, the total number of symmetries is 2, with 3 basis functions for the first symmetry and 2 basis functions for the second. The key for translating the numbers in each box into the L, M, P, Q, R, and S values is given in the bottom left. Notice how all rows have the same M, R, and S values, while all columns have the same L, P, and Q values. For clarity, the boxes have been coloured, based on the spinor symmetries that they contain.

by substituting the relevant variables. If there is sufficient global memory available, these values can be stored and referred to later as needed. Otherwise, they could be calculated on the fly as needed. Because binary search scales as $\mathcal{O}(\log n)$, this should ensure that this



Figure 2.6: Two-electron integral matrix as a vector: The top triangle of the two-electron symmetric matrix in a vector representation. In this instance, the total number of symmetries is 2, with 3 basis functions for the first symmetry and 2 basis functions for the second. The key for translating the numbers in each box into the L, M, P, Q, R, and S values is given in the bottom center. Notice how the L, M, P, Q, R, and S values are much harder to predict than from the matrix representation. For clarity, the boxes have been coloured based on the spinor symmetries that they contain. Gaps between rows are used to reinforce that the elements are not connected like a matrix.

remains a fast method of mapping threads to integrals for large problems as well. With some alterations, this method could also apply to molecular symmetries and not only to a single atom. For instance in the C₁ symmetry, all possible combinations of four basis functions must be used (ignoring those that appear on the bottom triangle of the two electron integral matrix of course). We could simply remove the search for L and M, have the initial value of high in Algorithm 5 be the total number of basis functions, and remove the sum $(s_nprime(1:L-1)$ term from lownum.

From here, the new code for evaluating the integrals remains largely the same as the

Algorithm 4 Binary search for L

```
i = threadIdx.x + (blockIdx.x - 1) * blockDim.x
if i \leq i_{max} then
  low = 1
  high = s_nsym
  while low < high do
    mid = \frac{(low+high)}{(low+high)}
    lownum = 1 + \mathbf{sum}(s\_nprime(1:mid-1))
    highnum = lownum - 1 + s_nprime(mid)
    if (i \leq highnum) and (i \geq lownum) then
       L = mid
       exit
    else if y > highnum then
       low = mid + 1
    else if y < lownum then
       high = mid - 1
    end if
  end while
end if
```

Algorithm 5 Binary search for P and Q

```
i = threadIdx.x + (blockIdx.x - 1) * blockDim.x
if i \leq i_{max} then
  low = 1
  high = s_n bs(L)
  while low \leq high do
    mid = \frac{(low + high)}{(low + high)}
    lownum = \frac{2}{(mid-1)(mid-2)}{2} + mid + \mathbf{sum}(s\_nprime(1:L-1))
    highnum = lownum + mid - 1
    if (i < highnum) and (i > lownum) then
       P = mid
       exit
    else if y > highnum then
       low = mid + 1
    else if y < lownum then
       high = mid - 1
    end if
  end while
  Q = y - lownum + 1
end if
```

original, except for some minor changes to allow for more efficient global or shared memory access. We also use a process referred to as "grid-stride looping" where all these binary search algorithms have their if $i \leq i_{max}$ then removed, and then are placed within the following loop: for i = threadIdx.x + (blockIdx.x - 1) * blockDim.x to i_{max} , i += blockDim.x *gridDim.x do. If we know the occupancy of the algorithm on the GPU beforehand, we can launch exactly the number of blocks that will fill the GPU. This reduces the overhead of block swapping and lets us further eke out some performance.

2.4.2 Density Matrix Formation

The term in parenthesis in Equation 1.36 corresponds to the non-relativistic density matrix. But as we are interested in relativistic calculations, it will need to be altered. Firstly, because a relativistic wavefunction has both large and small components, so too does its density matrix. Therefore, it will have two dimensions that span from 1 to 2K where dimensions 1 to K are the large components and the rest are for small components. Secondly, the factor of 2 is replaced by the number of electrons that can occupy spinors of symmetry μ . The density matrix's matrix and vector representations are shown in Figures 2.7 and 2.8 respectively. The mathematical form of the density matrix is given in Equation 2.6[29]

$$\mathbf{D}_{\mathbf{C}r,s} = N_{\mu} \sum_{a=1}^{occ} \mathbf{C}_{r,a} \mathbf{C}_{s,a}^{*}$$
(2.6)

where N_i is the number of electrons that occupy a closed shell of symmetry *i*. **D**_O is similar to this and is shown below.

$$\mathbf{D}_{\mathbf{O}r,s} = N_i \mathbf{C}_{r,(occ+1)} \mathbf{C}^*_{s,(occ+1)}$$
(2.7)

where N_i is equal to the number of electrons in the open shell. Note that in this program, only the most energetic shell of any symmetry can be open.

The total density matrix is $D_T = D_C + D_O$

2.4.2.1 P and Q Supermatrices

With the density matrices in hand we can begin to combine the two-electron integrals from the previous section. These integrals have the following form.[29]

1 ^L 1 ^L 1	2 ^L 1 ^L 2	3 ^L 1 ^L 4	4 ^L 1 ^L 7	5 ^L 1 ^L 11	1 ⁸ 1 ^L 16	2 ⁸ 1 ^L 22	3 ^s 1 ^L 29	4 ⁸ 1 ^L 37	5 ⁸ 1 ^L 46
	2 ^L 2 ^L 3	3 ^L 2 ^L 5	4 ^L 2 ^L 8	5 ^L 2 ^L 12	1 ⁸ 2 ^L 17	2 ⁸ 2 ^L 23	3 ^s 2 ^L 30	4 ⁸ 2 ^L 38	5 ⁸ 2 ^L 47
		3 ^L 3 ^L 6	4 ^L 3 ^L 9	5 ^L 3 ^L 13	1 ⁸ 3 ^L 18	2 ⁸ 3 ^L 24	3 ^s 3 ^L 31	4 ⁸ 3 ^L 39	5 ⁸ 3 ^L 48
			4 ^L 4 ^L 10	5 ^L 4 ^L 14	1 ⁸ 4 ^L 19	2 ⁸ 4 ^L 25	3 ^s 4 ^L 32	4 ⁸ 4 ^L 40	5 ⁸ 4 ^L 49
				5 ^L 5 ^L 15	1 ⁸ 5 ^L 20	2 ⁸ 5 ^L 26	3 ⁸ 5 ^L 33	4 ⁸ 5 ^L 41	5 ⁸ 5 ^L 50
					1 ⁸ 1 ⁸ 21	2 ⁸ 1 ⁸ 27	3 ⁸ 1 ⁸ 34	4 ⁸ 1 ⁸ 42	5 ⁸ 1 ⁸ 51
						2 ⁸ 2 ⁸ 28	3 ⁸ 2 ⁸ 35	4 ^s 2 ^s 43	5 ⁸ 2 ⁸ 52
							3 ^s 3 ^s 36	4 ⁸ 3 ⁸ 44	5 ⁸ 3 ⁸ 53
								4 ⁸ 4 ⁸ 45	5 ⁸ 4 ⁸ 54
R ^x S ^x I									5 ⁸ 5 ⁸ 55

Figure 2.7: Density matrix as a matrix. The top triangle of the symmetric density matrix in a matrix representation. The key for translating the numbers in each box into the R and S values is given in the bottom right. All active symmetries would have a similar, separate matrix. For clarity, the elements have been colorized based on the combination of large and small components they contain.

1 ^L 1 ^L	2 ^L 1 ^L	2 ^L 2 ^L	3 ^L 1 ^L	3 ^L 2 ^L	3 ^L 3 ^L	4 ^L 1 ^L	4 ^L 2 ^L	4 ^L 3 ^L	4 ^L 4 ^L
1	2	3	4	5	6	7	8	9	10
5 ^L 1 ^L	5 ^L 2 ^L	5 ^L 3 ^L	5 ^L 4 ^L	5 ^L 5 ^L	1 ^S 1 ^L	1 ^S 2 ^L	1 ^S 3 ^L	1 ^S 4 ^L	1 ⁸ 5 ^L
11	12	13	14	15	16	17	18	19	20
1 ^s 1 ^s	2 ^S 1 ^L	2 ^S 2 ^L	2 ^S 3 ^L	2 ^s 4 ^L	2 ^S 5 ^L	2 ^s 1 ^s	2 ^S 2 ^S	3 ^s 1 ^L	3 ^s 2 ^L
21	22	23	24	25	26	27	28	29	30
3 ⁸ 3 ^L	3 ⁸ 4 ^L	3 ^S 5 ^L	3 ^s 1 ^s	3 ^s 2 ^s	3 ^s 3 ^s	4 ^s 1 ^L	4 ⁸ 2 ^L	4 ^s 3 ^L	4 ^s 4 ^L
31	32	33	34	35	36	37	38	39	40
4 ^s 5 ^L	4 ⁸ 1 ⁸	4 ^S 2 ^S	4 ^S 3 ^S	4 ^s 4 ^s	5 ^s 1 ^L	5 ^S 2 ^L	5 ⁸ 3 ^L	5 ⁸ 4 ^L	5 ⁸ 5 ^L
41	42	43	44	45	46	47	48	49	50
5 ^S 1 ^S									

Figure 2.8: Density matrix as a vector. The top triangle of the symmetric density matrix in a vector representation. The key for translating the numbers in each box into the R and S values is given in the bottom left. All active symmetries would have a similar, separate vector that continue one after the other. For clarity, the elements have been colorized based on the combination of large and small components they contain.

$$\begin{aligned} \mathbf{X}_{I(pqrs)}^{1} &= (p_{L}q_{L}|r_{L}s_{L}) - \frac{1}{2} \left[(p_{L}r_{L}|q_{L}s_{L}) + (p_{L}s_{L}|q_{L}r_{L}) \right] \\ \mathbf{X}_{I(pqrs)}^{2} &= (p_{L}q_{L}|r_{S}s_{S}) \\ \mathbf{X}_{I(pqrs)}^{3} &= (p_{S}q_{S}|r_{L}s_{L}) \\ \mathbf{X}_{I(pqrs)}^{4} &= - (p_{L}r_{S}|q_{S}s_{L}) \\ \mathbf{X}_{I(pqrs)}^{5} &= - (p_{L}s_{S}|q_{S}r_{L}) \\ \mathbf{X}_{I(pqrs)}^{5} &= - (p_{S}r_{L}|q_{L}s_{S}) \\ \mathbf{X}_{I(pqrs)}^{7} &= - (p_{S}s_{L}|q_{L}r_{S}) \\ \mathbf{X}_{I(pqrs)}^{7} &= - (p_{S}q_{S}|r_{S}s_{S}) - \frac{1}{2} \left[(p_{S}r_{S}|q_{S}s_{S}) + (p_{S}s_{S}|q_{S}r_{S}) \right] \end{aligned}$$
(2.8)

where the subscripts L and S refer to the large and small components respectively. I is a function that returns the values of x and y from Equations 2.2 and 2.3 where $L = \lambda$ and $M = \mu$. From here, all subscripts of **X** will be implied to go through this I function.

The \mathbf{P} and \mathbf{Q} super matrices have a similar layout to the density matrices. The elements of \mathbf{P} have the following form[29]

$$\mathbf{P}_{pq}^{LL} = \sum_{\mu=1}^{nsym} \sum_{r=1}^{msym} \sum_{s=1}^{msym} \left(\mathbf{D}_{\mathbf{T}rs}^{LL} \mathbf{X}_{pqrs}^{1} + \mathbf{D}_{\mathbf{T}rs}^{SS} \mathbf{X}_{pqrs}^{J(pqrs)} \right)$$

$$\mathbf{P}_{pq}^{SS} = \sum_{\mu=1}^{nsym} \sum_{r=1}^{msym} \sum_{s=1}^{msym} \left(\mathbf{D}_{\mathbf{T}rs}^{SS} \mathbf{X}_{pqrs}^{8} + \mathbf{D}_{\mathbf{T}rs}^{LL} \mathbf{X}_{pqrs}^{J(pqrs)} \right)$$

$$\mathbf{P}_{pq}^{LS} = \sum_{\mu=1}^{nsym} \sum_{r=1}^{msym} \sum_{s=1}^{msym} \left(\mathbf{D}_{\mathbf{T}rs}^{LS} \mathbf{X}_{pqrs}^{5} + \mathbf{D}_{\mathbf{T}rs}^{SL} \mathbf{X}_{pqrs}^{J(pqrs)} \right)$$

$$\mathbf{P}_{pq}^{SL} = \sum_{\mu=1}^{nsym} \sum_{r=1}^{msym} \sum_{s=1}^{msym} \left(\mathbf{D}_{\mathbf{T}rs}^{SL} \mathbf{X}_{pqrs}^{7} + \mathbf{D}_{\mathbf{T}rs}^{LS} \mathbf{X}_{pqrs}^{J(pqrs)} \right)$$
(2.9)

where J(pqrs) is an integer function that selects specific definitions of the two-electron integrals from Equation 2.8. How exactly this works is shown in the following sections.

The form of the \mathbf{Q} super matrix is almost the same a \mathbf{P} , but there will be an additional multiplication of the vector coupling coefficient between the open shells for each summation.

2.4.2.2 FORMPQ Algorithm

Forming the P and Q matrices proved to be the most difficult part of this program to parallelize. Its difficulty was due to the second term in the summations where each \mathbf{X} matrix used depends on how far the summation has progressed. Further, each element of

P will have the **X** matrix change at different times. These two factors result in many **if** statements which GPUs have difficulty handling in parallel. There is also the issue where each element in the LL and SS sections need to loop over every element of the same sections of the density matrix, as do the LS and SL sections. This means that there will be lots of global memory reads unless handled properly. All together, this makes for a very ugly algorithm to parallelize.

Two different attempts were made to try and accelerate this algorithm. Each tried to exploit a different property of GPUs. One attempted to combat the amount of floating point operations to perform by distributing the amount of work to as many threads as possible. This will be referred to as the Multiple Threads Single Element (MTSE) algorithm. The second one tried to deal with the amount of global memory reads by making the most of each read. This will be referred to as Single Thread Single Element (STSE) algorithm. Each will be described in the sections below.

2.4.2.3 MTSE Algorithm

As previously stated, the purpose of the MTSE algorithm is to distribute the amount of work needed to be done to as many threads as possible. This was achieved by having multiple threads each computing two of the multiplications needed for a single element of two matrices in Equation 2.9, and then combining the products of these multiplications in parallel. These two tasks were performed by two separate kernels. Pseudocode showing how each calculates the \mathbf{P} matrix is shown in Algorithms 6 and 7 respectively.

inttype refers to one or more of the **P** or **Q** matrices. In Algorithm 6, inttype can have a value of 0 or 1, where 0 refers to the *LL* and *SS* **P** or **Q** matrices, and 1 is the *SL* and *LS* matrices. In Algorithm 7, inttype can have a values ranging from 0 to 7 where 0 to 3 are the **P** *LL*, *SS*, *SL*, *LS* matrices, and the rest are the **Q** matrices in the same order. *d* is **D** in its vector representation and *pos* are the locations of the *p* and *q* elements within it. *locmx* is an array with 7 elements, and each element is equal to the number of unique *LL*, *SS*, *SL*, *LS* elements of symmetry l - 1. fctr accounts for when an element is single or double counted in the summation. $x(\chi, :)$ is the vector representation of \mathbf{X}^{χ} , *loc* is the location of needed pqrs element in the vector, total is the length of one of the dimensions of \mathbf{X}^{χ} , and k1 and k2 are the outputs of the *J* function from Equation 2.9. Finally, *pXY* variables are matrices dimension total × total and store the sum of the two multiplications of the *d* and *x* vectors, *pmx* if the vector representation of the *P* matrices, and *s_tile* is a vector in the shared memory for summing up the elements of each row of the *pXY* matrices.

The grid will need to have $\frac{total-1}{blockDim.x} \times \frac{total-1}{blockDim.y} \times 2$ dimensions for Algorithm 6 and $\frac{total-1}{blockDim.x} \times \frac{total-1}{blockDim.y} \times 8$ for Algorithm 7. Algorithm 6 is fairly straightforward, but Algorithm 7 could use a little more explanation. It is a "parallel reduction" algorithm. At the start, each

Algorithm 6 Kernel 1 for MTSE

```
i = threadIdx.x + (blockIdx.x - 1) * blockDim.x
j = blockIdx.y
inttype = blockIdx.z - 1
if i \leq total then
  l = lpq\_array(i, 1)
  p = lpq\_array(i, 2)
  q = lpq_array(i, 3)
  fctr = 1.0
  if (p \neq q) and (inttype == 0) then
     fctr = 2.0
  else if (p == q) and (inttype == 1) then
    fctr = 0.5
  end if
  loc = \max(i, j) + ((\max(i, j) - 1) * (\max(i, j) - 2)/2) + \min(i, j) - 1
  if (inttype == 0) then
    if i > j then
       k1 = 3
       k2 = 2
    else
       k1 = 2
       k2 = 3
    end if
    pos1 = locmx(l) + ((p-1)^2 + p - 1)/2 + q
    pos2 = locmx(l) + ((p - 1 + nbs(l))^{2} + p + nbs(l) - 1)/2 + q + nbs(l)
    pLL(i, j) = d(pos1) * fctr * x(1, loc) + d(pos2) * fctr * x(k1, loc)
    pSS(i, j) = d(pos1) * fctr * x(k2, loc) + d(pos2) * fctr * x(k8, loc)
  else
    if i > j then
       k1 = 4
       k2 = 6
    else
       k1 = 6
       k^{2} = 4
    end if
    pos1 = locmx(l) + ((p - 1 + nbs(l))^2 + p - 1 + nbs(l))/2 + q
    pos2 = locmx(l) + ((q - 1 + nbs(l))^{2} + q - 1 + nbs(l))/2 + p
    pSL(i, j) = d(pos1) * fctr * x(7, loc) + d(pos2) * fctr * x(k1, loc)
    pLS(i, j) = d(pos1) * fctr * x(k2, loc) + d(pos2) * fctr * x(5, loc)
  end if
end if
```

Algorithm 7 Kernel 2 for MTSE

```
i = threadIdx.x + (blockIdx.x - 1) * blockDim.x * 2
inttype = blockIdx.z - 1
if inttype == 0 then
  if i \leq total then
    s_tile(threadIdx.x) = pLL(i, blockIdx.y)
  else
    s_tile(threadIdx.x) = 0.0
  end if
  if i + blockDim.x \leq total then
    s_tile(threadIdx.x + blockDim.x) = pLL(i + blockDim.x, blockIdx.y)
  else
    s_tile(threadIdx.x + blockDim.x) = 0.0
  end if
else
  Perform a similar instruction on the other pXY or qXY matrices depending on inttype
```

```
end if
for j = \log_2(blockDim.x), j \ge 0, j = j - 1 do
  call syncthreads
  if threadIdx.x \leq 2^{j} then
     s\_tile(threadIdx.x) = s\_tile(threadIdx.x) + s\_tile(threadIdx.x + 2^{j})
  end if
end for
if threadIdx.x == 1 then
  l = lpq\_array(blockIdx.y, 1)
  p = lpq_array(blockIdx.y, 2)
  q = lpq\_array(blockIdx.y, 3)
  if (inttype == 0) then
    pos = locmx(l) + ((p-1)^2 + p - 1)/2 + q
    istat = \mathbf{atomicadd}(pmx(pos), s\_tile(threadIdx.x))
  else
    Perform a similar instruction on the other pXY or qXY matrices depending on inttype
  end if
end if
```

thread loads an element of the relevant pXY array into the shared variable s_tile and also loads the element that is blockDim.x elements ahead of the original element. Then, in a loop starting from $j = \log_2(blockDim.x)$ and descending to j = 0 threads with a threadIdx.xvalue of less then 2^j add the value of $s_tile(threadIdx.x + 2^j)$ to $s_tile(threadIdx.x)$. The key feature is that the amount of elements that need to be added is reduced by half in every loop. Because it is possible that the total number of elements of pXY needed to sum up for the relevant pmx element could be larger than one block can handle, atomic operations are used to force the final addition to occur serially.

2.4.2.4 STSE Algorithm

The STSE algorithm tries a different approach to this problem than the MTSE algorithm. Instead of trying to spread out the amount of work to do as much as possible, it tries to reduce the amount of global memory reads by making each thread do as much work as it can. This results in fewer blocks, but each block needs to run longer. Giving only the calculations for pmx and when inttype = 0, Algorithm 8 shows how this is done.

All variables are the same as in Algorithms 6 and 7, but *inttype* can only be 0 or 1 (the meanings are the same as in Algorithm 6). As for the new variables, s_d is a chunk of d that has been loaded into the shared memory. *mink* and *maxk* are used to calculated the sections of x that current chunk of d in shared memory applies to and *loop* is used to adjust the value of *loc* if the needed two-electron integral is on the bottom triangle of a **X** matrix. *pm*1 and *pm*2 are accumulator variables that track the sum of an element of *pmx* as d is looped through.

Algorithm 8 has two nested loops. The outer one loops over elements of d, loading chunks of it into the shared memory as it goes. The inner one loops over elements of x and performs the multiplications of d and x elements, keeping a running tally of the sum of these multiplications. Something that is not shown in the pseudocode is checking if l and m have open shells. If both of them do, then qm1 and qm2 will be calculated as well. If only one or neither of them do, then this calculation is skipped. Because most of the shells will be closed, this allows for many calculations to be skipped. Once the inner loop has finished, the next section of d is loaded into the shared memory and then the multiplication of x and s_{-d} continues. This process goes on until all elements of a row of \mathbf{X} have been used.

2.5 Discussion

In this section, the results of GPU resource usage and profiling the various algorithms discussed previously will be presented. For profiling, the radon atom was chosen. Radon was selected because it contains many spinor orbitals and should be a good test of the **formpq**

Algorithm 8 STSE algorithm

```
i = threadIdx.x + (blockIdx.x - 1) * blockDim.x
inttype = blockIdx.z - 1
if i < total then
     l = lpq\_array(i, 1)
     p = lpq_array(i, 2)
     q = lpq\_array(i,3)
      fctr = 1.0
     loop = 0
     for j = 1, j \le (total - 1)/blockDim.x + 1, j = j + 1 do
           mink = 1 + (j - 1) * blockDim.x
           maxk = \min(j * blockDim.x, total)
           if threadIdx.x + (j-1) * blockDim.x < total then
                 m = lpq\_array(threadIdx.x + (j - 1) * blockDim.x, 1)
                 r = lpq_array(threadIdx.x + (j-1) * blockDim.x, 2)
                 s = lpq\_array(threadIdx.x + (j - 1) * blockDim.x, 3)
                 if (r \neq s) and (inttype == 0) then
                       fctr = 2.0
                 end if
                 s_d(threadIdx.x, 1) = fctr * d(locmx(m) + ((r-1)^2 + r - 1)/2 + s - 1)
                 s_d(threadIdx.x, 2) = fctr * d(locmx(m) + ((r-1+nbs(m))^2 + r + nbs(m) - 1)/2 + nbs(m) -
                 s + nbs(m)
           end if
           fctr = 1.0
           call syncthreads
           for k = mink, k \le maxk, k = k + 1 do
                 if (i \ge k) and (inttype == 0) then
                      loc = ((i-1)^2 + i - 1)/2 + k
                      k1 = 3
                      k2 = 2
                 else if (i < k) and (inttype == 0) then
                      loop = loop + k - 1
                      loc = (i^2 + i)/2 + loop
                      k1 = 2
                      k2 = 3
                 end if
                 pm1 = pm1 + s_d(1 + k - mink, 1) * x(1, loc) + s_d(1 + k - mink, 2) * x(k1, loc)
                 pm2 = pm2 + s_d(1 + k - mink, 1) * x(k2, loc) + s_d(1 + k - mink, 2) * x(k8, loc)
           end for
           call syncthreads
     end for
     pmx(locmx(l) + ((p-1)^2 + p - 1)/2 + q) = pm1
     pmx(locmx(l) + ((p - 1 + nbs(l))^2 + p + nbs(l) - 1)/2 + q + nbs(l)) = pm2
end if
```

and *eint2* kernels on large atomic systems. Some of the smaller basis sets used do not contain a sensible number of basis functions considering the number of electrons that Radon contains. This is not an issue though, as at this stage we are only concerned with how long the calculation takes, and not with how accurate its end result is. Therefore, basis sets use the arbitrarily chosen WTBS parameters of $\alpha = 6.87 \times 10^{-2}$, $\beta = 1.83$, $\delta = 3.97$, and $\gamma = 0.78$. Additionally, due to the spherical symmetry of an atom exploited by cudaDFRATOM, the growth of a calculation differs depending on how the basis functions are distributed among the spinor symmetries. Therefore, results are reported in terms of the number of two-electron integrals instead of number of basis functions as is typically done.

2.5.1 Resource Usage

In the case of the work in this thesis, the resource bottleneck for my kernels was almost always the number of registers used per thread. 63 32-bit registers provide only 252 bytes to work with, which when using double precision 8-byte numbers is hardly anything at all. A summary of the block sizes and resource usage of all kernels is given in Table 2.1.

Kernel	Block Size	Registers	Shared Memory (bytes)
eint1	(512, 1, 1)	63	45056
eint2	(512, 1, 1)	63	45088
vec2matrix	(512, 1, 1)	17	0
formd	(512, 1, 1)	33	28672
$binary_search$	(512, 1, 1)	30	60
convd	(512, 1, 1)	25	0
MTSE	(512, 1, 1)	46	32768
STSE	(512, 1, 1)	56	39388
forme	(512, 1, 1)	39	4152
form f	(512, 1, 1)	18	0
xtrpf	(512, 1, 1)	12	0
formg	(32, 16, 1)	55	12288
swapcol	(32, 16, 1)	10	0

 Table 2.1: Kernel resource usage

Of these kernels, eint2 and the $formpq_alg$ kernels take up the bulk of the time needed in a typical calculation. This is in part due to the exponential growth in the number of twoelectron integrals, but it is also caused by the amount of register spilling that each kernel will have. As stated in Section 2.2.2 when the amount of registers a thread needs exceeds the amount that is available, it will begin to store the data in the global memory. As global memory is the slowest available memory type, this is very undesirable. To counteract this, many variables that would otherwise be better stored in register memory were moved into the shared memory. But this is also undesirable because it means that there will be less shared memory available for storing data that needs to be read frequently from global memory. This in turn leads to more frequent reads from the global memory. Solving this balancing act required many iterations of testing, moving variables around, compiling, and retesting. Eventually, I arrived at the configurations shown above. Note how each kernel uses a block containing 512 threads. This number was chosen because it is the largest possible block size that can run when the required number of register per thread exceeds 32. 512 is also a good block size because in instances where a kernel is not limited by register or shared memory usage, it allows for the maximum number of threads per SM (1536) to be run.

2.5.2 Two-Electron Integral performance

Table 2.2 and Figure 2.9 show the results of profiling the *eint2* kernel against its CPU counterpart.

Table 2.2: *eint2* kernel performance. Times are in ms. Times given are an average of five runs.

Two- Electron Integrals ^a	CPU Time	eint2	$binary_search$	Total GPU time	Speedup ^b	Speedup ^c
74305	59	4.68	0.18	4.86	12.81	12.32
353220	320	18.03	0.71	18.74	17.72	17.04
1081185	980	52.50	2.21	54.71	18.66	17.90
2588950	2360	118.26	5.36	123.62	19.96	19.09
5299140	4910	237.75	11.07	248.82	20.63	19.71
9726255	8880	437.74	20.81	458.55	20.27	19.35
16476670	15140	730.56	35.96	766.52	20.73	19.75
26248635	24180	1160.82	58.00	1218.82	20.84	19.85

^a For only the upper triangle of one of the eight \mathbf{X} matrices.

^b Speedup comparing just the time of *eint2* to the CPU time.

^c Speedup comparing the time of *eint2* and *binary_search* to the CPU time.

As can be seen, the GPU calculations of the two-electron integrals outperform the CPU calculations with an average speedup factor of over 19. For calculations with fewer number of integrals to compute the speedup is not as dramatic. This is most likely due to the overhead involved in just starting a GPU kernel. Table 2.2 shows two different speedups: one for just calculation of the integrals, and one that shows the speedup if the time needed



Figure 2.9: Profiling of two-electron Integral calculations. The results of profiling the calculation of growing amounts of two-electron integrals. The blue line shows the time needed for GPU calculations and the yellow line shows time needed for CPU calculations. The time for the GPU calculations is the combined time of the **eint2** and **binary_search** kernels.

for **binary_search** is included. The time needed to evaluate indices does not have much of an impact on the total performance on the total calculation time which proves this was a good way to generate the *lmpqrs* indices. Additionally, because cudaDFRATOM is a basis set optimizer, **binary_search** will need to be called only once, whereas **eint2** may need to be called many hundreds of times. Therefore, for an optimization calculation (which the original program is incapable of doing) the total speedup will limit to the just the integral calculations.

2.5.3 P and Q Matrix Formation Performance

As explained in section 2.4.2.1, there were two different attempts to speedup the formation of **P** and **Q**. The results of these attempts are shown in Tables 2.3 and 2.4 and also in Figure 2.10.

As can be seen, the attempt at **MTSE** was a complete failure and it isn't even faster than the CPU calculations. **STSE** was much better, but only just. It achieves little more than a two-fold speedup at best.

Two-Electron Integrals	Time per Iteration CPU	Time per Iteration GPU	Speedup
74305	1.90	6.06	0.31
353220	5.78	14.25	0.40
1081185	18.42	27.81	0.66
2588950	39.47	53.95	0.73
5299140	81.05	96.13	0.84
9726255	152.50	173.64	0.87
16476670	266.53	291.79	0.91
26248635	426.25	459.38	0.92

Table 2.3: *MTSE* kernel profiling results. Times are in ms. Times are given as the average time needed for a single iteration from one calculation.

Table 2.4: *STSE* kernel profiling results. Times are in ms. Times are given as the average time needed for a single iteration from one calculation.

Two-Electron Integrals	Time per Iteration CPU	Time per Iteration GPU	Speedup
74305	1.90	2.94	0.64
353220	5.78	7.56	0.76
1081185	18.42	15.34	1.20
2588950	39.47	26.32	1.49
5299140	81.05	39.45	2.05
9726255	152.50	88.78	1.71
16476670	266.53	135.64	1.96
26248635	426.25	193.99	2.19

There are several reasons this could be the case. The first due to the poor global memory access that reading x has. x is stored as a vector. This helps greatly with memory cost and integral calculation, but makes it difficult to retrieve it as if it were a matrix. There is the cost of calculating where the necessary integral is, and then the cost of the very uncoalesced reads. Calculating the integrals as a vector, and then copying them into a matrix afterwards could help with this, but the large amount of integrals needed for large calculations makes this impractical on current hardware. How much of an effect inefficient access of global memory has on a calculation does have a limit however which is most likely why the speedup sees an improvement as the calculations get larger. A second reason that the speedup is limited is caused by the occupancy that the kernels can achieve on the GPU. A block size of 512 means that there is a maximum number of 3 blocks running per SM at a time. But these kernels are both limited by the register usage to just running one block per SM at a time. This is also most likely why MTSE performs so poorly compared STSE. MTSE



Figure 2.10: Profiling of the formpq kernels. The results of profiling the formation of the P and Q matrices. The blue line shows the time needed for GPU calculations using the MTSE algorithm, the yellow line shows time needed for GPU calculations using STSE, and the green line shows the time needed for the CPU. Because the GPU calculations converge in fewer SCF iterations than the CPU calculations, only the average time for one iteration is shown.

was designed to spread out the amount of work to as many threads as possible. This results in a lot of blocks to be run. But because the amount of blocks that can run at a time is so limited there is no chance to see an improvement. But in the case of **STSE**, there are a fewer number of blocks needing be be run, although each one needs to run for longer than those of **MTSE**. Overall **MTSE** comes out on top.

At present, the limitations of these algorithms are caused by the hardware they run on, not the efficiency of the algorithms themselves. If we imagine removing these limitations, we could consider which one will be better. I propose that MTSE will eventually surpass STSE for very large systems for the following reasons: the time it takes for a single block of MTSE to run is mostly governed by how well it can read the x vector. The effect of spreading out the elements has on memory bandwidth has a limit, once the elements are spread out enough, spreading them out further has no impact. Therefore there is a maximum amount of time it takes for a single block to run. The time for a single block of STSE on



Figure 2.11: Integrals needed for the first element of P: The top triangle of the symmetric two-electron integral matrix in a matrix representation. The required integrals have been highlighted with a green border. The basis set used had nsym = 3 with nbs(i) = (10, 10, 10). For clarity, the boxes have been coloured based on the spinor symmetries that they contain.



Figure 2.12: Integrals needed for the first element of P: The top triangle of the symmetric two-electron integral matrix in a vector representation. The required integrals have been highlighted with a green border. The spreading out of the elements means that reads to them can not be done effectively. The basis set used had nsym = 3 with nbs(i) = (10, 10, 10). For clarity, the boxes have been coloured in the same way as Figure 2.11.

the other hand is controlled by both the efficiency of reading global memory and the amount of two-electron integrals it must read though. So there is no limit to how long a block can take. Therefore, I predict that MTSE should be faster as the number of integrals becomes very large.

2.5.4 Total Speedup

There was some difficulty in determining the total speedup of a calculation. The reason why can be seen in Tables 2.5 and 2.6.

Table 2.5: Total speedup of cudaDFRATOM using **MTSE**. The results for a total calculation are shown. All times are in s. Times are given as the average time needed for five calculations.

Two-Electron Integrals	SCF Iterations CPU	Total CPU Time	SCF Iteractions GPU	Total GPU Time	Speedup
74305	21	0.12	21	0.84	0.14
353220	19	0.49	19	1.19	0.41
1081185	19	1.44	19	1.75	0.82
2588950	19	3.38	19	2.58	1.30
5299140	19	6.78	19	3.80	1.78
9726255	24	13.29	19	5.77	2.30
16476670	26	23.23	19	8.60	2.69
26248635	24	35.63	19	12.5	2.82

Table 2.6: Total speedup of cudaDFRATOM using **STSE**. The results for a total calculation are shown. All times are in s.

Two-Electron Integrals	SCF Iterations CPU	Total CPU Time	SCF Iteractions GPU	Total GPU Time	Speedup
74305	21	0.12	21	0.78	0.15
353220	19	0.49	19	1.07	0.46
1081185	19	1.44	19	1.51	0.95
2588950	19	3.38	19	2.08	1.62
5299140	19	6.78	19	2.72	2.49
9726255	24	13.29	19	4.14	3.20
16476670	26	23.23	19	5.57	4.16
26248635	24	35.63	19	7.47	4.76



Figure 2.13: Total time need to complete a calculation.

As can be seen, the number of SCF iterations differs when comparing the GPU calculations to the CPU even though the convergence criteria was exactly the same. This is somewhat puzzling but I offer the following explanation. The differences do not occur in the two-electron integral calculations. We confirmed this by comparing the sum of the absolute values of the integrals from both the GPU and non-GPU programs and found that they were the same. The problem instead occurs as a result of changing the SCF routines. First, when writing the SCF routines, it became apparent that rewriting the linear algebra into CUDA would be rather pointless when I could just use the cuSOLVER and cuBLAS libraries and achieve the same result. As such, the SCF is completed using entirely different algorithms and unfortunately, these GPU libraries do not produce exactly the same eigenvalues as the original program. Second, it is important to realize that a real number can only be approximated using double precision variables. This introduces numerical instability. For instance, assume that we have a computer that could only hold the first four digits of a number (leading zeros don't count). Then we take the number 1.000 and we want to add 0.0001000 to it 10000 times. The result of the first addition should be 1.0001, but because our computer can only hold four digits, the number is truncated to 1.000. The final result of this computation would not be 2.000 as expected but 1.000. During an SCF calculation, there are millions of numbers being multiplied together and added up, many of which may be close to, but not quite 0. This allows for lots of error to creep into a calculation just because of the limitations of the hardware.

The fact that two different algorithms are being used on the GPU and CPU, and that they might not be handling numerical stability in the same way is what is most likely causing this to occur. It should also be pointed out that the final energy was not exactly the same from GPU to CPU either. Typically, the last 4 of 16 significant digits would be different. Because the rest are the same however, we still have "chemical accuracy" (the general consensus of chemical accuracy is 0.001 Hartree, which cudaDFRATOM falls well within) and I argue that cudaDFRATOMs results are therefore valid.

2.6 Input Description

cudaDFRATOM can be executed on Unix-like systems in the following way

```
$ path_to_executable input_file > output_file
```

The input file must end in ".inp" or an error will be given. Redirection of stdout to an output file is optional, but is recommended to save the results of a calculation. The input file is read using the namelist functionality of Fortran. A description of what must appear on each line of the input file is given below. Sample input files are also given in Appendix A.

- 1. A title of no more than 200 characters.
- 2. \$contrl

'energy'	Will do a single point energy calculation.
'bsopt'	Will optimize the basis set. Can only be
	used if bastype equals 'wtbs'.
	The speed of light. If not given, the de-
	fault is set to 137.03599976 au.
	'energy' 'bsopt'

3. \$nuc

znuc			The charge of the nucleus.
nucmdl			The nuclear model to use.
	=	1	Point nucleus (default).
	=	2	Finite sphere (not yet supported).
	=	3	Gaussian.
rnuc			The radius of the finite sphere nucleus.
alpha			The exponent for the gaussian nucleus.
-			Defaults are given in litdata.f90.

4. \$bas

nsym			The number of symmetries to be used.
bastype			The type of basis set given.
	=	'wtbs'	Use a WTBS basis set.
	=	'rdin'	Read in the basis set from the input file.
ngroup			The number of different groups to use in
			the WTBS scheme (default 1).

The next line will depend on the value of bastype. If bastype equals 'rdin' then the following lines must be the number of functions for the S+ symmetry, followed by the exponents to use, each on a new line. The pattern repeats for each new symmetry. See the sample input files for further clarification. Otherwise, if bastype equals 'WTBS' the \$wtbs group is read next.

5. \$wtbs has to be given if bastype='wtbs'.

wtbspara	The α , β , δ , and γ WTBS parameters. If
	there is more than one group, the order
	would be $\alpha_1, \beta_1, \delta_1, \gamma_1, \alpha_2, \beta_2, \delta_2, \gamma_2$ and
	so on.
nbs	The number of functions used in each sym-
	metry.
start	Where in the ζ pool each symme-
	try starts taking exponents from (de-
	fault=1,1,1,1,1,1,1).
groups	What group each symmetry belongs to
	(default=1,1,1,1,1,1,1).

The next line depends on what the jobtype was set to. If jobtype equals 'energy' \$newuoa is skipped and \$econfig will be read next. If jobtype equals 'bsopt', then the \$newuoa group will be needed.

6. \$newuoa has to be given if jobtype='bsopt'. Refer to the newuoa documentation [32] for detailed information if needed.

rhobe	g			The initial value of the trust region used has maximum $(def with 0.1)$
rhoen	d			by newuoa (default=0.1). The final value of the trust region used by newuoa. Must be smaller than rhobeg $(default=1.0 \times 10^{-4})$
inrint				$(\text{default}-1.0 \times 10^{\circ})$. The print level for newwood
ipimo		_	0	No printing from newuoa (default)
		_	1	Print only when newuoa has finished
		=	2	Print only when the trust region has de-
			_	creased by an order of magnitude.
		=	3	Print every iteration of newuoa.
maxfu	ın			The maximum number of calls to calfun
				newuoa will make before terminating (de-
				fault=500).
7. \$econfi	g			
nclose))			The number of closed spinors for each symmetry
nopen	1			The number of open spinors for each sym-
1				metry. There is a limit to one open orbital
				per symmetry.
freeel				The number of electrons available in the
				open spinors.
autog	en			Automatically generates all possible com-
-				binations of spinor occupancies (de-
				fault=.false.).
nconf				The number of configurations to be read
				in (needed if autogen is false).
If autogen is false, then the next near lines will be the spinor occupancies				

If autogen is false, then the next nconf lines will be the spinor occupancies. They will be given as real numbers with one configuration per line.

8. \$scf

		The maximum number of SCF iterations (default=50).
		The method of extrapolation.
=	0	No extrapolation (default).
=	1	Extrapolate the Fock matrix.
		Damping factor for Fock maxtrix (de-
		fault=0.3).
		Convergence limit for the large-large
		components of the density matrix
		$(\text{default}=1.0 \times 10^{-5})$
		Convergence limit for the small-large
		components of the density matrix
		$(\text{default}=1.0 \times 10^{-7})$
		Convergence limit for the small-small
		components of the density matrix
		$(\text{default}=1.0 \times 10^{-9})$
		$ = 0 \\ = 1 $

Chapter 3

Basis Sets

3.1 Introduction

As stated in section 1.2.2, the use of Gaussian-type functions is the favored way of constructing basis sets for the use in molecular calculations. The use of basis sets introduces a new source of error, as we are now only approximating a wavefunction instead of directly numerically calculating it. One of the ways this error can manifest itself is in basis set superposition error (BSSE). BSSE appears when comparing the differences in energy between two different systems, as one might do to compare the difference in energy between reactants and product in a chemical reaction.

For instance, we might want to find the energy of the reaction $H^+ + OH^- \rightarrow H_2O$. The calculation of H_2O will have three basis functions centers while the OH^- calculation will only have two. The OH^- fragment inside the H_2O molecule will have additional basis functions from the H^+ fragment to work with while the OH^- does not. As a result, the OH^- fragment and molecule are not being described exactly the same, and therefore errors can result from this.

There is also the possibility of approximate linear dependencies in the basis set, which may show up during the SCF process. This happens when the overlap between any two different functions is close to unity (at least as far as a double precision number is concerned) and will mean that there will be eigenvalues that are equal to zero when diagonalizing the overlap matrix. We cannot find the inverse of such a matrix, so therefore the functions leading to these eigenvalues of zero must get transformed out of the matrix. This is kind of bandaid solution though, as the resulting Fock matrix after this transformation could produce errors in the energy differences on the order of chemical accuracy. It can also lead to a very aggravating process during a geometry optimization.

For example, say we have a molecular system in geometry state A. In this state, there are no approximate linear dependencies, and the geometry optimizer determines that the system would prefer to be in geometry state B. It updates the geometry, but in state B, some atoms might be too close together and now there are eigenfunctions that need to be rejected. The energy calculated for geometry state B is inaccurate, which causes the geometry optimizer to think that it should place the atoms back into state A. But now, everything is exactly the same as it was, and the geometry optimizer, with no memory at all of what just happened, thinks that the perfect geometry is state B again. There is no way out of this loop, and we will not be able to find a stationary state, and all because of a poor choice in basis set. It is therefore important for a computational chemist to be aware of these issues so they can identify them when they occur, but even more so for someone who wants to make a new basis set, so that these issues can be avoided in the first place.

Designing a basis set that reduces the effects of BSSE is relatively straightforward, we can simply brute force the problem by adding more and more functions until they begin to cancel each other out. Designing one that avoids the issue of approximate linear dependencies however is more tricky. It is simply not possible to test every possible combination of atoms in every possible geometry to determine if a basis set has these problems. But there are some strategies we can use to avoid this problem.

One strategy that has shown to be particularly effective is using an exponent generating function to ensure that the exponents of the basis set are sufficiently different. There are many of these generating functions. One of these gives what are called even-tempered basis sets (ETBS)[33]. The generating function for an ETBS is given below

$$\zeta_{l,k} = \alpha_l \beta_l^{k-1}, \quad \alpha_l, \beta_l > 0, \quad \beta_l \neq 1, \quad k = 1, 2, \dots$$

$$(3.1)$$

where $\zeta_{l,k}$ is the k^{th} exponent of basis function for orbital symmetry l, α_l is the exponent for the first, most diffuse, basis function, and β_l is a growth parameter that determines the gap between $\zeta_{l,k}$ and $\zeta_{l,k+1}$. This greatly reduces the difficulty of the problem, because instead of needing to optimize all the exponents of our basis set, we only need to optimize the α and β parameters of each symmetry. We can further reduce the number of parameters to optimize by using the same α and β parameters for each symmetry. This is what I did for the work in this chapter, so I will drop the l subscript. However, there is a problem with ETBS: the growth in the value of the exponents is not always sufficient. So we get diminishing returns by increasing the maximum value of k, and we have to add many more functions to improve the accuracy of the basis set by even a small amount. This is improved in the well-tempered basis set (WTBS)[34] generating function, which is shown below

$$\zeta_k = \zeta_{k-1} \beta \left[1 + \gamma \left(\frac{k}{n} \right)^{\delta} \right], \quad k = 2, 3, \dots, n, \quad \zeta_1 = \alpha$$
(3.2)

where n is the maximum number of basis functions for the set, and α and β have the same



Figure 3.1: Changes in ζ as the values of δ and γ are changed. The value of n was 36, α was 0.02, and β was 1.5

restrictions on them as they did before. The parameters δ and γ have the effect of increasing the gap between ζ s caused by β at high k. This means that the growth of the exponents is increased as they get larger, which allows them to make a more meaningful contribution to the total wavefunction. Thus, we get a more accurate basis set with far fewer functions. The effect that altering γ and δ has on the exponents can be seen in Figure 3.1.

It should be mentioned that each symmetry does not need to use the entire set of ζ s that we optimize. Indeed, the most diffuse orbitals in the valence shells often don't use the most contracted functions at all, and conversely the most contracted orbitals in the core don't make much use of the most diffuse functions. Therefore, it is better to think of the set of ζ s as pool, and that each symmetry is drawing a range of functions from that pool.

3.2 Methods

3.2.1 Basis set size optimization

We decided to use a somewhat novel method of generating our basis sets. We begin by choosing an arbitrarily large basis set size, such as s(1:40)p(1:40)d(1:40)f(1:40) (here

i(#:#) refers to the starting and ending index of ζ 's used for symmetry *i*). Next, we then find the optimal α , β , δ , and γ WTBS parameters for this basis set. This is done using NEWUOA[32] which finds the values α , β , δ , and γ that lead to the lowest possible energy for a given basis set size. Finally, we use the following steps to find the optimal basis set size.

Step 1. Begin by finding the fewest number of f functions necessary. This can be done by generating input files that range in size from s(1:40)p(1:40)d(1:40)f(1:1) to s(1:40)p(1:40)d(1:40)f(1:40).

Step 2. Optimize the basis sets and select the smallest basis set that is still below some minimum accuracy threshold. We chose a relative error to numerical calculations of no greater than 5.0×10^{-9} for non-relativistic sets and 5.0×10^{-8} for relativistic sets where relative error is defined as $\frac{|(\text{optimized energy})-(\text{numerical energy})|}{\text{numerical energy}}$. The size of this basis set is $s(1:40)p(1:40)d(1:40)f(1:x_f)$.

Step 3. Replace the WTBS parameters with those from the newly optimized set and generate a list of input files that range in size from $s(1:40)p(1:40)d(1:x_f)f(1:x_f)$ to $s(1:40)p(1:40)d(1:40)f(1:x_f)$.

Step 4. Optimize these new sets and select the smallest one that brings about an error that is still below the accuracy threshold. The size of this basis set is $s(1:40)p(1:40)d(1:x_d)f(1:x_f)$.

Step 5. Repeat steps 3 and 4 for the remaining symmetries. The size of the basis set at the end of this step will be of size $s(1:x_s)p(1:x_p)d(1:x_d)f(1:x_f)$.

Step 6. Replace the WTBS parameters with those from the newly optimized set and generate a list of input files that range in size from $s(1:x_s)p(1:x_p)d(1:x_d)f(1:x_f)$ to $s(1:x_s)p(1:x_p)d(1:x_d)f(x_f:x_f)$.

Step 7. Optimize and select from the basis sets. The new set will be of size $s(1:x_s)p(1:x_p)d(1:x_d)f(y_f:x_f)$.

Step 8. Repeat steps 6 and 7 for the other symmetries except s. The final basis set will be of size $s(1:x_s)p(y_p:x_p)d(y_d:x_d)f(y_f:x_f)$.

This procedure is perhaps a bit clunky, so let us work through an example using Ne. Ne has both s and p type orbitals, and so will our basis set. We might initially guess that no more than 26 functions per symmetry will enough to get the accuracy we want, so we start with a basis set of size s(1:26)p(1:26). We then optimize the α , β , δ , and γ parameters for a basis set of this size. We make sure that the energy using a basis set of this size produces results that are accurate enough, and then we begin to reduce the size of the basis set for the p space. We carry over the WTBS parameters optimized in the last step, and generate input files corresponding to basis sets of size s(1:26)p(1:15) to s(1:26)p(1:26) (12 calculations in total) to determine the minimum number of tight functions we will need to
accurately describe the p orbitals. After reoptimizing the WTBS parameters, we find that while s(1:26)p(1:15) is too small to be accurate enough, s(1:26)p(1:16) is still inside the threshold we want. So, we take the WTBS parameters from this calculation, and use them to generate new basis sets ranging in size from s(1:16)p(1:16) to s(1:26)p(1:16) (so we are trying to eliminate contracted functions from the s orbitals). Here we find that s(1:23)p(1:16) is the smallest basis set we can use. Now, we want to eliminate diffuse functions. Carrying over the WTBS parameter from the last acceptable basis set, we generate basis sets of size s(1:23)p(1:16) to s(1:23)p(5:16). We find that trying to remove any more functions makes the basis set unacceptable so we keep the s(1:23)p(1:16) basis set. We could try to remove diffuse functions from the s symmetry, but experience teaches that the s space needs all the functions to be accurate, so we don't bother.

This process has a major drawback in that it requires a lot of computer power to run efficiently. But this is not really a problem if access to large computer clusters is available. Additionally, considering that calculations for the chain 1-8 can be run in parallel for different atoms, this optimization process is trivially parallel. The advantages of this process are twofold: it finds a very small basis set that is still accurate and it is completely automatable. If there are no problems with individual calculations not converging, the output files never even need to be manually (and intellectually) examined! We generated non-relativistic basis sets for elements 2-86 using the rWTBS program[34–39] and relativistic basis sets for elements 55-86 using the cudaDFRATOM program which is outlined in detail in Chapter 2.

3.2.2 Automating Optimization

Automating the optimization process was quite simple. I did this by writing two scripts: BS_sub_auto_rwtbs.sh and BS_find_best_rwtbs.sh. The code for BS_sub_auto.sh is given here

```
1 #!/bin/bash
2
3 sym=''
4 alljobs=false
5 bottom=false
6 path_to_exe='/some/path' # must be set!
7 wtime=01:00:00
8
9 if [[ -z $path_to_exe ]]; then
10 echo "You must set the path to rwtbs.exe"
11 exit
12 fi
13
14 while [ $# -gt 0 ]
15 do
16 val=$1
```

```
shift
17
     case $val in
18
       "-a")
19
           alljobs=true
20
        ;;
21
       "-b")
22
          bottom=true
23
24
       ;;
       "-S")
           sym='S'
26
           low=$1
27
28
           high=$2
           shift
29
           shift
30
        ;;
31
       "-P")
32
           sym='P'
33
           low=$1
34
           high=$2
35
           shift
36
           shift
37
         ;;
38
         "-D")
39
           sym='D'
40
           low=$1
41
           high=$2
42
           shift
43
           shift
44
45
         ;;
        "-F")
46
           sym='F'
47
           low=$1
48
           high=$2
49
           shift
50
           shift
51
52
         ;;
        "-t")
53
           wtime=$1
54
           shift
56
         ;;
        *)
57
           job=$val
58
59
        ;;
     esac
60
61 done
62
63
```

```
64 boilerplate(){
65 cat << EOF
66 #!/bin/bash
67 #SBATCH --account=def-mariusz # change depending
68 #SBATCH --mem=2GB
69 #SBATCH --time=$1
70 #SBATCH --job-name=$2
71
72 echo -----
73 echo -----
74 echo began running on \'date\'
75 echo -----
76 echo -----
77 $3/rwtbs $2 >& $4
78 echo -----
79 echo -----
80 echo stopped running on \'date\'
81 echo -----
82 echo -----
83 EOF
<sub>84</sub> }
85
86
87 if [ "$alljobs" == true ]; then
se job='ls *inp'
89 elif [ -z "$job" ]; then
90 echo no job given
91 exit
92 fi
93
94 for file in $job; do
   dir=$(echo $file | sed -e "s/-.*//")
   if [[ -d "$dir" ]]; then
96
     echo "$dir already here"
   else
98
     mkdir $dir
99
   fi
   cd $dir
   # keep old out files and delete others
   rename "out" "out-old" *.out
   rm *inp
   rm *GUS
   rm *MCS
108
   cp ../$file $file"-orig"
109
   file_base=$(echo $file | sed -e 's/_.*//')
110
```

```
# read the number of basis functions
    read -r -a old_bs <<< $(sed -n -e '/nbfsym/{s/.*nbfsym(1)=//; s/\$end//; p}'</pre>
      $file"-orig")
     # get the most contracted basis function
     IFS='+' read -r -a old_top <<< $(sed -n -e '/ +/p' $file"-orig")
     # keep track of how many files are made
117
     total=0
118
     for i in $(seq $low $high); do
119
       for j in $(seq 0 3); do
         new_bs[j]=${old_bs[j]}
         new_top[j]=${old_top[j]}
       done
124
       # make alterations based on symmetry
       case $sym in
126
         "F")
           ((new_bs[3]-=$i))
           # make sure that not too many functions are cut
           if [[ "${new_bs[3]}" == "0" ]]; then
             break
           fi
           ((new_top[3]+=$i))
           ;;
         "D")
           ((new_bs[2]-=$i))
           if [[ "${new_bs[2]}" == "0" ]]; then
             break
           fi
139
           ((new_top[2]+=$i))
140
141
           ;;
         "P")
           ((new_bs[1]-=$i))
143
           if [[ "${new_bs[1]}" == "0" ]]; then
144
             break
145
           fi
146
           ((new_top[1]+=$i))
147
           ;;
148
         "S")
149
           ((new_bs[0]-=$i))
           if [[ "${new_bs[0]}" == "0" ]]; then
             break
           fi
           ((new_top[0]+=$i))
154
           ;;
       esac
156
```

```
# make new calculation
158
      new_file=$file_base"_"${new_bs[0]}"s"${new_bs[1]}"p"${new_bs[2]}"d"${new_bs[3]}"f.inp"
      cp $file"-orig" $new_file
      sed -i "s/nalp=${old_bs[0]}/nalp=${new_bs[0]}/" $new_file
161
      sed -i "s/${old_bs[0]} ${old_bs[1]} ${old_bs[2]} ${old_bs[3]}/${new_bs[0]}
      ${new_bs[1]} ${new_bs[2]} ${new_bs[3]}/" $new_file
      if [ "$bottom" == false ]; then
        sed -i -e "s/${old_top[0]}+/${new_top[0]} +/" -e
      "s/${old_top[1]}+/${new_top[1]} +/" -e "s/${old_top[2]}+/${new_top[2]} +/" -e
      "s/${old_top[3]} +/${new_top[3]} +/" $new_file
      fi
166
      # write submission script
      boilerplate $wtime $new_file $path_to_exe ${new_file%???}out >
      ${new_file%???}.sh
      #sbatch ${new_file%???}.sh # uncomment to automatically submit job
       ((total++))
    done
    echo "$total files made"
    cd ../
  done
```

Listing 3.1: *BS_sub_auto_rwtbs.sh*

The first few lines handle the arguments given to the script. The arguments are flags which tell the script what to do. The flags can be given in any order, so long as each flag is followed by the appropriate options. The default flag is a file ending in ".inp" for the calculation that you would like to run. Optionally, this flag can be omitted, which will tell the script to run over all "inp" files in the current directory. I will refer to the input file to be used as a seed. The flags "-S", "-P", "-D", and "-F" tell the script which set of orbitals we would like to remove functions from ("-S" means s orbitals, "-P" means p orbitals, and so on). These flags <u>must</u> be followed by by two integers, with the first being smaller than the second. The first number is the minimum number for functions to cut, and the second is the maximum number to cut. By default, cutting begins with the most contracted function. For example, using "-S 0 3" would take the seed file with a basis set of size s(1:20) and produce otherwise identical files with basis sets of size s(1:20), s(1:19), s(1:18), and s(1:17). If the number are negative, this can be used to add basis functions ("-S -1 0" on the same seed would produce basis sets of size s(1:21) and s(1:20)). Using the "-B" (for bottom) flag changes the default behavior of cutting contracted functions, to cutting diffuse functions. So for example, using the flags "-S 0 3 -B" on the seed would produce s(1:20), s(2:20), s(3:20), and s(4:20).

Once the flags have been parsed, the script makes a directory with the same name as the title of the seed, moves inside this directory, and generates the needed input files. It also creates a job submission script using the boilerplate function for each of new input files and submits them. Note that this part of the script will need to be changed depending on the cluster it is being used on. If more than one seed is used, then the script will do the same thing for each seed. After the jobs are completed, the user runs BS_find_best_rwtbs.sh in the directory that contains all of the newly created directories. The code for BS_find_best_rwtbs.sh is given below

```
#!/bin/bash
  tol=$1
  if [ -z $tol ]; then
    tol='5*10^-9'
  fi
7
  echo The tolerance in relative error is $tol
 mkdir best
11
  for dir in 'ls -d */'; do
    if [ "$dir" != 'old/' ]; then
      if [ "$dir" != 'best/' ]; then
        if [ "$dir" != 'tests/' ]; then
        cd $dir
        for file in *.out; do
          error='grep -A 1 '[E(WT)-E(rf)]/E(rf)' $file | tail -1 | awk '{print
     $4}''
          comperror='echo $error | sed -e 's/D/\*10\^/'
          testthress=$(bc -1 <<< "scale=20; ($tol - $comperror)*10^10 >= 1")
          if [ $testthress -ge 1 ]; then
21
            cp 'echo $file | sed -e 's/out/inp/' .../best
            cp $file ../best
23
            echo Found best for $file
24
            break
          fi
26
        done
        fi
      fi
    fi
30
    cd ..
  done
```

Listing 3.2: BS_find_best_rwtbs.sh

This script takes in one argument, the relative error we are looking for in a calculation. It enters each of the subdirectories made by BS_sub_auto.sh and scans the output files for the relative error compared to numerical calculations. It finds the file with the smallest basis set that is still under the error threshold, and copies the input and output files for that calculation into a new directory called "best". The user can then repeat this process for as many orbitals as they wish. There are also similar scripts for cudaDFRATOM which are given in Appendix B.

3.3 Discussion

3.3.1 Optimized Non-Relativistic Basis Sets

The optimized non-relativistic WTBS parameters and basis set sizes for elements 2-86 are shown in Table 3.1. Relativistic WTBS parameters for elements 55-86 are shown in Table 3.2. Table 3.3 gives the energies calculated with these basis sets compared to their literature values.

Table 3.1: Basis sets optimized using rWTBS. We did not have literature data for some elements. These elements are marked with a *. The size of the basis set for these elements was determined by using the size of the nearest elements.

Element	Term	α	β	δ	γ	s	р	d	f
	Symbol								
02 He	^{1}S	8.140×10^{-2}	1.953	4.504	1.515	(1:18)			
03 Li	^{2}S	1.596×10^{-2}	1.933	5.701	1.573	(1:22)			
04 Be	^{1}S	2.647×10^{-2}	1.938	5.841	1.594	(1:22)			
$05 \mathrm{B}$	^{2}P	3.238×10^{-2}	1.948	5.573	1.523	(1:22)	(1:15)		
06 C	^{3}P	4.613×10^{-2}	1.941	4.717	1.317	(1:23)	(1:15)		
07 N	4S	5.976×10^{-2}	1.923	5.183	1.442	(1:23)	(1:16)		
08 O	^{3}P	6.967×10^{-2}	1.936	5.170	1.426	(1:23)	(1:16)		
09 F	^{2}P	8.321×10^{-2}	1.942	5.084	1.408	(1:23)	(1:16)		
10 Ne	^{1}S	9.943×10^{-2}	1.945	4.988	1.392	(1:23)	(1:16)		
11 Na	^{2}S	1.696×10^{-2}	1.950	6.056	1.469	(1:26)	(3:19)		
$12 { m Mg}$	^{1}S	2.375×10^{-2}	1.932	5.686	1.430	(1:26)	(3:19)		
13 Al	^{2}P	2.239×10^{-2}	1.898	5.555	1.413	(1:27)	(1:20)		
$14 \mathrm{Si}$	^{3}P	3.352×10^{-2}	1.921	5.419	1.410	(1:26)	(1:19)		
15 P	4S	4.410×10^{-2}	1.907	5.196	1.390	(1:26)	(1:19)		
$16 \mathrm{S}$	^{3}P	5.004×10^{-2}	1.896	4.962	1.362	(1:26)	(1:19)		
17 Cl	^{2}P	5.831×10^{-2}	1.886	4.784	1.344	(1:26)	(1:19)		
18 Ar	^{1}S	6.834×10^{-2}	1.878	4.654	1.331	(1:26)	(1:19)		
19 K	^{2}S	1.392×10^{-2}	1.889	6.354	1.523	(1:28)	(3:22)		
$20 \mathrm{Ca}$	^{1}S	1.837×10^{-2}	1.874	6.109	1.504	(1:28)	(3:22)		
$21 \ Sc$	^{2}D	2.040×10^{-2}	1.878	6.160	1.505	(1:28)	(3:22)	(2:16)	
22 Ti	${}^{3}F$	2.218×10^{-2}	1.886	6.247	1.508	(1:28)	(3:22)	(2:16)	
$23 \mathrm{V}$	${}^{4}F$	2.361×10^{-2}	1.887	6.573	1.507	(1:29)	(3:23)	(2:16)	

 Table 3.1: (continued)

Element	Term Symbol	α	eta	δ	γ	S	р	d	f
24 Cr	7S	2.345×10^{-2}	1.865	5.348	1.407	(1:29)	(3:22)	(2:17)	
$25 { m Mn}$	6S	2.572×10^{-2}	1.865	5.336	1.407	(1:29)	(3:22)	(2:17)	
26 Fe	^{5}D	2.621×10^{-2}	1.869	5.301	1.395	(1:29)	(3:22)	(3:17)	
27 Co	${}^{4}F$	2.643×10^{-2}	1.871	5.905	1.413	(1:29)	(4:23)	(3:17)	
28 Ni	${}^{3}F$	2.882×10^{-2}	1.875	5.935	1.413	(1:29)	(3:23)	(3:17)	
29 Cu	^{2}S	2.283×10^{-2}	1.857	5.485	1.413	(1:30)	(4:23)	(3:18)	
30 Zn	^{1}S	3.297×10^{-2}	1.881	5.817	1.339	(1:30)	(3:24)	(2:17)	
31 Ga	^{2}P	2.742×10^{-2}	1.863	5.703	1.462	(1:30)	(1:23)	(3:18)	
32 Ge	^{3}P	3.143×10^{-2}	1.848	5.290	1.386	(1:30)	(1:23)	(4:18)	
$33 \mathrm{As}$	4S	4.728×10^{-2}	1.869	5.325	1.340	(1:30)	(1:23)	(3:17)	
$34 { m Se}$	^{3}P	5.087×10^{-2}	1.847	4.949	1.533	(1:30)	(1:22)	(3:18)	
35 Br	^{2}P	5.927×10^{-2}	1.861	5.192	1.333	(1:30)	(1:23)	(3:17)	
36 Kr	^{1}S	6.804×10^{-2}	1.859	5.510	1.370	(1:29)	(1:23)	(3:17)	
37 Rb	^{2}S	1.421×10^{-2}	1.856	7.181	1.626	(1:30)	(3:25)	(6:21)	
38 Sr	^{1}S	1.808×10^{-2}	1.846	6.674	1.553	(1:30)	(3:25)	(6:20)	
39 Y	^{2}D	1.997×10^{-2}	1.841	6.569	1.543	(1:30)	(3:25)	(2:20)	
40 Zr	${}^{5}F$	2.184×10^{-2}	1.837	6.485	1.535	(1:30)	(3:25)	(2:20)	
41 Nb	^{6}D	2.340×10^{-2}	1.835	6.434	1.530	(1:30)	(3:25)	(2:20)	
42 Mo	^{7}S	2.537×10^{-2}	1.832	6.372	1.524	(1:30)	(3:25)	(2:20)	
43 Tc	6S	2.597×10^{-2}	1.836	6.453	1.534	(1:30)	(3:25)	(2:20)	
44 Ru	${}^{5}F$	2.682×10^{-2}	1.833	6.788	1.606	(1:30)	(3:25)	(2:21)	
45 Rh	${}^{4}F$	2.751×10^{-2}	1.835	6.883	1.620	(1:30)	(3:25)	(2:21)	
46 Pd	^{1}S	5.944×10^{-2}	1.827	5.980	1.504	(1:29)	(2:24)	(1:19)	
47 Ag	^{2}S	2.438×10^{-2}	1.800	5.521	1.423	(1:31)	(4:25)	(3:21)	
48 Cd	^{1}S	2.911×10^{-2}	1.786	5.334	1.408	(1:31)	(4:25)	(3:21)	
49 In	^{2}P	2.714×10^{-2}	1.799	5.540	1.431	(1:31)	(1:25)	(3:21)	
$50~{ m Sn}$	^{3}P	2.884×10^{-2}	1.794	5.422	1.415	(1:31)	(1:25)	(4:21)	
$51~{ m Sb}$	4S	4.481×10^{-2}	1.815	6.567	1.605	(1:30)	(1:25)	(3:21)	
52 Te	^{3}P	4.846×10^{-2}	1.817	6.247	1.528	(1:30)	(1:26)	(3:20)	
53 I	^{2}P	5.369×10^{-2}	1.810	6.016	1.505	(1:30)	(1:25)	(3:20)	
54 Xe	^{1}S	5.981×10^{-2}	1.802	5.862	1.490	(1:30)	(1:25)	(3:20)	
$55~\mathrm{Cs}$	^{2}S	1.177×10^{-2}	1.792	6.485	1.510	(1:33)	(4:28)	(5:23)	
56 Ba	^{1}S	1.560×10^{-2}	1.770	6.152	1.518	(1:32)	(3:28)	(6:23)	
57 La	^{2}D	1.716×10^{-2}	1.764	6.067	1.513	(1:32)	(3:28)	(2:23)	(5:14)
58 Ce^*	^{3}H	1.652×10^{-2}	1.774	6.254	1.529	(1:32)	(3:28)	(2:23)	(4:19)
59 Pr	^{4}I	$1.696\!\times\!10^{-2}$	1.776	6.297	1.533	(1:32)	(3:28)	(6:23)	(4:19)
60 Nd	^{5}I	$1.737{ imes}10^{-2}$	1.778	6.563	1.579	(1:32)	(3:28)	(6:24)	(4:19)
61 Pm	^{6}H	1.784×10^{-2}	1.780	6.615	1.585	(1:32)	(3:28)	(6:24)	(4:19)
$62~\mathrm{Sm}$	^{7}F	$1.857{ imes}10^{-2}$	1.778	5.842	1.464	(1:33)	(3:27)	(6:23)	(4:19)
63 Eu	^{8}S	1.876×10^{-2}	1.784	6.718	1.596	(1:32)	(3:28)	(6:24)	(4:19)

Table 3.1: (continued)

Element	Term Symbol	α	β	δ	γ	S	р	d	f
64 Gd*	^{7}F	1.926×10^{-2}	1.782	6.844	1.599	(1:33)	(3:28)	(6:24)	(4:19)
65 Tb^*	^{6}H	1.971×10^{-2}	1.784	6.898	1.604	(1:33)	(3:28)	(6:24)	(4:19)
66 Dy	^{5}I	2.020×10^{-2}	1.788	6.543	1.540	(1:33)	(3:28)	(6:23)	(4:19)
67 Ho*	^{4}I	2.064×10^{-2}	1.785	7.090	1.640	(1:33)	(3:28)	(6:23)	(4:20)
68 Er	^{3}H	2.106×10^{-2}	1.792	7.029	1.638	(1:32)	(3:28)	(6:24)	(4:20)
$69~\mathrm{Tm}$	^{2}F	2.152×10^{-2}	1.794	7.075	1.643	(1:32)	(3:28)	(6:24)	(4:20)
70 Yb^*	^{1}S	2.200×10^{-2}	1.795	7.141	1.652	(1:32)	(3:28)	(2:24)	(4:20)
71 Lu	^{2}D	2.373×10^{-2}	1.790	7.018	1.640	(1:32)	(3:28)	(2:24)	(4:20)
$72 \ \mathrm{Hf}$	${}^{3}F$	2.511×10^{-2}	1.788	6.963	1.636	(1:32)	(3:28)	(2:24)	(5:20)
73 Ta	${}^{4}F$	2.684×10^{-2}	1.784	6.907	1.633	(1:32)	(2:28)	(2:24)	(5:20)
$74 \mathrm{W}$	^{5}D	2.814×10^{-2}	1.783	6.889	1.633	(1:32)	(3:28)	(2:24)	(5:20)
$75 { m Re}$	6S	2.931×10^{-2}	1.782	6.886	1.634	(1:32)	(3:28)	(2:24)	(5:20)
76 Os	^{5}D	3.075×10^{-2}	1.781	6.896	1.637	(1:32)	(2:29)	(2:24)	(4:20)
$77 \ {\rm Ir}$	${}^{4}F$	3.195×10^{-2}	1.780	6.867	1.635	(1:32)	(3:28)	(2:24)	(5:20)
78 Pt	^{3}D	3.173×10^{-2}	1.785	7.020	1.654	(1:32)	(3:28)	(2:24)	(5:20)
79 Au	^{2}S	3.190×10^{-2}	1.791	6.702	1.569	(1:33)	(4:28)	(2:23)	(5:19)
$80 { m ~Hg}$	^{1}S	3.546×10^{-2}	1.781	6.691	1.604	(1:32)	(3:28)	(2:23)	(5:20)
81 Tl	^{2}P	3.241×10^{-2}	1.794	6.826	1.561	(1:34)	(1:29)	(3:23)	(6:20)
$82 \ Pb$	^{3}P	3.867×10^{-2}	1.778	6.948	1.656	(1:32)	(1:28)	(3:25)	(6:21)
83 Bi	4S	4.514×10^{-2}	1.766	6.158	1.545	(1:32)	(1:27)	(2:24)	(6:19)
84 Po	^{3}P	4.783×10^{-2}	1.763	5.977	1.516	(1:32)	(1:27)	(3:23)	(6:19)
85 At	^{2}P	5.210×10^{-2}	1.757	5.846	1.502	(1:32)	(1:27)	(3:23)	(6:19)
$86 \mathrm{Rn}$	^{1}S	$5.716 imes 10^{-2}$	1.749	5.695	1.486	(1:32)	(1:27)	(3:23)	(6:19)

 Table 3.2: Basis sets optimized using cudaDFRATOM

Element	Electron Configuration	α	β	δ	γ	S	р	d	f
	Conngulation								
$55 \mathrm{Cs}$	$[Xe] 6s^1$	1.824×10^{-2}	1.921	6.085	1.062	(1:29)	(3:28)	(5:20)	
56 Ba	$[Xe] 6s^2$	2.033×10^{-2}	1.904	5.473	1.161	(1:30)	(3:28)	(6:20)	
57 La	$[Ba] 4f^1$	1.540×10^{-2}	1.871	5.166	2.036	(1:33)	(4:28)	(5:22)	(4:16)
$58 { m Ce}$	$[Ba] 4f^2$	1.838×10^{-2}	1.857	4.969	1.450	(1:31)	(3:28)	(5:22)	(4:16)
$59 \mathrm{Pr}$	$[Ba] 4f^3$	1.945×10^{-2}	1.857	4.947	1.438	(1:31)	(3:28)	(5:22)	(4:16)
60 Nd	$[Ba] 4f^4$	2.043×10^{-2}	1.859	4.928	1.422	(1:31)	(3:28)	(5:22)	(4:16)
$61 \mathrm{Pm}$	$[Ba] 4f^5$	2.142×10^{-2}	1.860	4.906	1.405	(1:31)	(2:28)	(4:22)	(4:16)
$62 \mathrm{Sm}$	$[Ba] 4f^6$	2.414×10^{-2}	1.856	4.854	1.379	(1:31)	(3:28)	(5:22)	(3:16)
63 Eu	$[Ba] 4f^7$	1.993×10^{-2}	1.877	5.099	1.020	(1:31)	(4:29)	(5:22)	(4:16)
$64 \mathrm{Gd}$	$[Ba] 4f^8$	2.063×10^{-2}	1.880	5.064	0.996	(1:31)	(4:29)	(5:22)	(4:16)
$65 \mathrm{Td}$	$[Ba] 4f^9$	$2.396\!\times\!10^{-2}$	1.869	4.840	0.967	(1:31)	(3:29)	(5:22)	(4:16)

β δ d f Element Electron α \mathbf{S} р γ Configuration $[Ba] 4f^{10}$ 66 Dy 2.177×10^{-2} 1.888 (5:22)5.3530.839(1:30)(4:29)(4:16) $[Ba] 4f^{11}$ 2.517×10^{-2} 67 Ho 1.878 5.1260.816 (1:30)(3:29)(5:22)(4:16)68 Er $[Ba] 4f^{12}$ 2.811×10^{-2} 1.875 5.1451.045(1:30)(3:29)(5:22)(3:16) $[Ba] 4f^{13}$ 2.628×10^{-2} 69 Tm1.887 5.4800.886(1:31)(3:30)(5:22)(4:16)70 Yb $[Ba] 4f^{14}$ 2.918×10^{-2} 1.883 5.490(5:22)0.873(1:31)(3:30)(3:16)71 Lu $[Yb] 5d^1$ 3.424×10^{-2} 1.873 5.1241.353(1:32)(2:29)(1:23)(3:16) $[Yb] 5d^2$ 3.982×10^{-2} 72 Hf 1.900 6.117 1.473(1:32)(2:29)(1:22)(4:16) 4.271×10^{-2} $[Yb] 5d^3$ 73 Ta 1.899 6.1261.450(1:32)(3:29)(1:22)(4:16) $[Yb] 5d^4$ 4.564×10^{-2} 1.901 $74 \mathrm{W}$ 5.9361.351(1:32)(3:29)(1:21)(4:16) 4.827×10^{-2} $[Yb] 5d^5$ 1.900 75 Re 5.8981.323(3:29)(1:21)(1:32)(4:16)76 Os $[Yb] 5d^6$ 5.081×10^{-2} 1.899 1.296 5.873(1:32)(3:29)(1:21)(4:16) $77 \mathrm{Ir}$ $[Yb] 5d^7$ 5.333×10^{-2} 1.898 1.2745.846(1:32)(3:29)(1:21)(4:16)78 Pt $[Yb] 5d^8$ 5.391×10^{-2} 1.892 6.0581.365(1:32)(3:29)(1:23)(5:16) $[Yb] 5d^9$ 79 Au 5.684×10^{-2} 1.893 6.1111.354(1:32)(3:29)(1:23)(5:16) $[Yb] 5d^{10}$ 5.965×10^{-2} 80 Hg 1.893 6.1561.342(3:29)(1:32)(1:23)(5:16) $[Hg] 6p^1$ 4.071×10^{-2} 81 Tl 1.875 5.1610.944(1:22)(1:30)(1:29)(5:17) 4.364×10^{-2} 82 Pb $[Hg] 6p^2$ 1.869 5.0150.925(1:30)(1:29)(3:22)(6:17)83 Bi $[Hg] 6p^3$ 5.109×10^{-2} 1.854 3.953 0.792(1:33)(1:30)(2:21)(5:17)84 Po $[Hg] 6p^4$ 5.439×10^{-2} 1.849 4.6660.890 (1:30)(1:29)(3:22)(6:17)85 At $[Hg] 6p^5$ 6.177×10^{-2} 1.892 10.2231.500(1:30)(1:31)(3:22)(6:16) $[Hg] 6p^6$ 6.671×10^{-2} 1.831 86 Rn 3.906 0.867 (1:31)(1:29)(3:21)(6:17)

 Table 3.2: (continued)

Table 3.3: Energies produced from basis sets in Tables 3.1 and 3.2. Relativistic basis sets are labeled with r. All energies are in Hartree. Non-relativistic data comes from [40]. Relativistic data comes from [27].

Element	Calculated Energy	Literature Energy	Absolute Error	Relative Error
02 He	-2.861	-2.861	$> 1 \times 10^{-6}$	3.6×10^{-9}
03 Li	-7.432	-7.432	$> 1 \times 10^{-6}$	2.9×10^{-9}
$04 \mathrm{Be}$	-14.573	-14.573	$> 1 \times 10^{-6}$	3.2×10^{-9}
05 B	-24.529	-24.529	$> 1 \times 10^{-6}$	4.8×10^{-9}
06 C	-37.688	-37.688	$> 1 \times 10^{-6}$	4.1×10^{-9}
07 N	-54.400	-54.400	$> 1 \times 10^{-6}$	2.8×10^{-9}
08 O	-74.809	-74.809	$> 1 \times 10^{-6}$	3.4×10^{-9}
09 F	-99.409	-99.409	$> 1 \times 10^{-6}$	4.0×10^{-9}
$10 {\rm Ne}$	-128.547	-128.547	1×10^{-6}	4.4×10^{-9}
11 Na	-161.858	-161.858	1×10^{-6}	4.4×10^{-9}
$12 { m Mg}$	-199.614	-199.614	1×10^{-6}	3.9×10^{-9}
13 Al	-241.876	-241.876	1×10^{-6}	2.8×10^{-9}

Element	Calculated Energy	Literature Energy	Absolute Error	Relative Error
14 Si	-288.854	-288.854	1×10^{-6}	4.6×10^{-9}
15 P	-340.718	-340.718	1×10^{-6}	4.3×10^{-9}
16 S	-397.504	-397.504	2×10^{-6}	4.5×10^{-9}
17 Cl	-459.482	-459.482	2×10^{-6}	4.6×10^{-9}
18 Ar	-526.817	-526.817	2×10^{-6}	4.5×10^{-9}
19 K	-599.164	-599.164	3×10^{-6}	4.6×10^{-9}
$20 \mathrm{Ca}$	-676.758	-676.758	3×10^{-6}	3.8×10^{-9}
$21 \ Sc$	-759.735	-759.735	3×10^{-6}	4.3×10^{-9}
22 Ti	-848.405	-848.405	4×10^{-6}	4.9×10^{-9}
$23 \mathrm{V}$	-942.884	-942.884	4×10^{-6}	4.4×10^{-9}
$24 \mathrm{Cr}$	-1043.356	-1043.356	4×10^{-6}	4.1×10^{-9}
$25 { m Mn}$	-1149.866	-1149.866	6×10^{-6}	4.8×10^{-9}
26 Fe	-1262.443	-1262.443	6×10^{-6}	4.5×10^{-9}
$27 \mathrm{Co}$	-1381.414	-1381.414	6×10^{-6}	4.6×10^{-9}
28 Ni	-1506.870	-1506.870	7×10^{-6}	4.8×10^{-9}
29 Cu	-1638.963	-1638.963	6×10^{-6}	3.4×10^{-9}
30 Zn	-1777.848	-1777.848	9×10^{-6}	4.8×10^{-9}
$31~\mathrm{Ga}$	-1923.261	-1923.261	9×10^{-6}	4.5×10^{-9}
$32 { m Ge}$	-2075.359	-2075.359	7×10^{-6}	3.3×10^{-9}
$33 \mathrm{As}$	-2234.238	-2234.238	1×10^{-5}	4.8×10^{-9}
$34 { m Se}$	-2399.867	-2399.867	1×10^{-5}	4.4×10^{-9}
$35 \mathrm{\ Br}$	-2572.441	-2572.441	1×10^{-5}	4.8×10^{-9}
$36~{\rm Kr}$	-2752.054	-2752.054	1×10^{-5}	4.7×10^{-9}
$37 \mathrm{~Rb}$	-2938.357	-2938.357	1×10^{-5}	4.7×10^{-9}
$38 \mathrm{Sr}$	-3131.545	-3131.545	1×10^{-5}	4.4×10^{-9}
39 Y	-3331.684	-3331.684	1×10^{-5}	4.4×10^{-9}
$40 \mathrm{Zr}$	-3538.995	-3538.995	1×10^{-5}	4.4×10^{-9}
$41 { m ~Nb}$	-3753.597	-3753.597	1×10^{-5}	4.3×10^{-9}
$42 { m Mo}$	-3975.549	-3975.549	1×10^{-5}	4.5×10^{-9}
$43 \mathrm{Tc}$	-4204.788	-4204.788	2×10^{-5}	4.7×10^{-9}
$44 \mathrm{Ru}$	-4441.539	-4441.539	2×10^{-5}	4.5×10^{-9}
$45 \mathrm{Rh}$	-4685.881	-4685.881	2×10^{-5}	4.8×10^{-9}
46 Pd	-4937.921	-4937.921	2×10^{-5}	4.8×10^{-9}
$47 \mathrm{Ag}$	-5197.698	-5197.698	2×10^{-5}	4.3×10^{-9}
48 Cd	-5465.133	-5465.133	2×10^{-5}	4.2×10^{-9}
49 In	-5740.169	-5740.169	2×10^{-5}	4.6×10^{-9}
$50~\mathrm{Sn}$	-6022.931	-6022.931	2×10^{-5}	3.9×10^{-9}
$51~{\rm Sb}$	-6313.485	-6313.485	2×10^{-5}	4.4×10^{-9}
$52 { m Te}$	-6611.784	-6611.784	3×10^{-5}	4.8×10^{-9}
53 I	-6917.980	-6917.980	3×10^{-5}	4.6×10^{-9}
54 Xe	-7232.138	-7232.138	3×10^{-5}	4.3×10^{-9}

 Table 3.3: (continued)

Element	Calculated Energy	Literature Energy	Absolute Error	Relative Error
$55 \mathrm{Cs}$	-7553.933	-7553.933	2×10^{-5}	3.6×10^{-9}
56 Ba	-7883.543	-7883.543	3×10^{-5}	4.9×10^{-9}
$57 \mathrm{La}$	-8221.066	-8221.066	4×10^{-5}	4.8×10^{-9}
$58 { m Ce}$	-8566.919	-	-	-
$59 \mathrm{Pr}$	-8921.180	-8921.181	4×10^{-5}	4.9×10^{-9}
60 Nd	-9283.882	-9283.882	4×10^{-5}	4.8×10^{-9}
$61 \mathrm{Pm}$	-9655.098	-9655.098	4×10^{-5}	4.7×10^{-9}
$62 { m Sm}$	-10034.952	-10034.952	4×10^{-5}	4.4×10^{-9}
63 Eu	-10423.543	-10423.543	4×10^{-5}	4.7×10^{-9}
$64 \mathrm{Gd}$	-10820.617	-	-	-
$65~{ m Tb}$	-11226.568	-	-	-
66 Dy	-11641.452	-11641.452	5×10^{-5}	4.4×10^{-9}
$67 { m Ho}$	-12065.289	-	-	-
$68 \mathrm{Er}$	-12498.152	-12498.152	6×10^{-5}	4.8×10^{-9}
$69~\mathrm{Tm}$	-12940.174	-12940.174	6×10^{-5}	4.8×10^{-9}
$70 { m Yb}$	-13391.456	-	-	-
71 Lu	-13851.807	-13851.808	6×10^{-5}	4.7×10^{-9}
$72 \ \mathrm{Hf}$	-14321.249	-14321.249	6×10^{-5}	4.8×10^{-9}
73 Ta	-14799.812	-14799.812	$7 imes 10^{-5}$	4.9×10^{-9}
$74 \mathrm{W}$	-15287.546	-15287.546	7×10^{-5}	4.8×10^{-9}
$75 { m Re}$	-15784.533	-15784.533	$7 imes 10^{-5}$	4.9×10^{-9}
76 Os	-16290.648	-16290.648	8×10^{-5}	5.0×10^{-9}
$77 \ {\rm Ir}$	-16806.113	-16806.113	8×10^{-5}	5.0×10^{-9}
78 Pt	-17331.069	-17331.069	8×10^{-5}	5.0×10^{-9}
79 Au	-17865.399	-17865.400	8×10^{-5}	4.9×10^{-9}
$80 { m ~Hg}$	-18408.991	-18408.991	9×10^{-5}	5.0×10^{-9}
81 Tl	-18961.824	-18961.824	8×10^{-5}	4.6×10^{-9}
82 Pb	-19524.008	-19524.008	9×10^{-5}	4.9×10^{-9}
83 Bi	-20095.586	-20095.586	1×10^{-4}	5.0×10^{-9}
84 Po	-20676.500	-20676.500	9×10^{-5}	4.6×10^{-9}
$85 \mathrm{At}$	-21266.881	-21266.881	9×10^{-5}	4.5×10^{-9}
$86 \mathrm{Rn}$	-21866.772	-21866.772	9×10^{-5}	4.3×10^{-9}
$55 \ \mathrm{Cs}^r$	-7786.771	-7786.771	3×10^{-4}	4.6×10^{-8}
56 Ba^r	-8135.644	-8135.645	3×10^{-4}	4.7×10^{-8}
57 La^r	-8493.543	-8493.543	4×10^{-4}	4.8×10^{-8}
$58 \ \mathrm{Ce}^r$	-8860.997	-8860.997	4×10^{-4}	4.5×10^{-8}
$59 \ \mathrm{Pr}^r$	-9238.148	-9238.148	4×10^{-4}	4.6×10^{-8}
60 Nd^r	-9625.131	-9625.131	4×10^{-4}	4.8×10^{-8}
$61 \ \mathrm{Pm}^r$	-10022.094	-10022.095	5×10^{-4}	4.9×10^{-8}
$62 \ \mathrm{Sm}^r$	-10429.162	-10429.163	5×10^{-4}	4.8×10^{-8}
$63 \ \mathrm{Eu}^r$	-10846.504	-10846.505	4×10^{-4}	4.4×10^{-8}

 Table 3.3: (continued)

Element	Calculated Energy	Literature Energy	Absolute Error	Relative Error
$64 \mathrm{Gd}^r$	-11274.242	-11274.242	5×10^{-4}	4.7×10^{-8}
$65 \mathrm{Td}^r$	-11712.544	-11712.545	5×10^{-4}	4.3×10^{-8}
66 Dy^r	-12161.545	-12161.545	6×10^{-4}	4.9×10^{-8}
$67 \ \mathrm{Ho}^r$	-12621.412	-12621.413	5×10^{-4}	4.6×10^{-8}
$68 \ \mathrm{Er}^r$	-13092.269	-13092.270	6×10^{-4}	4.9×10^{-8}
$69 \ \mathrm{Tm}^r$	-13574.316	-13574.317	6×10^{-4}	4.8×10^{-8}
70 Yb^r	-14067.676	-14067.677	6×10^{-4}	$4.6 imes 10^{-8}$
$71 \ {\rm Lu}^r$	-14572.532	-14572.533	7×10^{-4}	4.9×10^{-8}
$72~{ m Hf}^r$	-15088.785	-15088.786	$7 imes 10^{-4}$	$4.9 imes 10^{-8}$
73 Ta^r	-15616.630	-15616.630	7×10^{-4}	4.7×10^{-8}
$74 \mathrm{W}^r$	-16156.184	-16156.185	8×10^{-4}	4.9×10^{-8}
$75 \ \mathrm{Re}^r$	-16707.619	-16707.620	8×10^{-4}	4.9×10^{-8}
76 Os^r	-17271.081	-17271.082	8×10^{-4}	4.9×10^{-8}
$77 \ \mathrm{Ir}^r$	-17846.787	-17846.788	8×10^{-4}	4.9×10^{-8}
$78 \ \mathrm{Pt}^r$	-18434.873	-18434.874	9×10^{-4}	$4.9 imes 10^{-8}$
79 Au^r	-19035.525	-19035.526	9×10^{-4}	4.9×10^{-8}
$80~{ m Hg}^r$	-19648.895	-19648.896	9×10^{-4}	$4.9 imes 10^{-8}$
81 Tl^r	-20274.849	-20274.850	9×10^{-4}	4.8×10^{-8}
82 Pb^r	-20913.713	-20913.714	9×10^{-4}	4.7×10^{-8}
83 Bi^r	-21565.705	-21565.706	1×10^{-3}	4.9×10^{-8}
84 Po^r	-22231.012	-22231.013	9×10^{-4}	4.1×10^{-8}
85 At^r	-22909.806	-22909.807	8×10^{-4}	3.7×10^{-8}
$86 \ \mathrm{Rn}^r$	-23602.103	-23602.104	1×10^{-3}	4.8×10^{-8}

 Table 3.3: (continued)

In Table 3.4 a comparison of the basis sets produced by cudaDFRATOM and Dyall's triple-zeta basis sets[41–43] is given. The cudaDFTAOM basis sets are all of similar accuracy as Dyall's basis sets for the 6s and 5d elements, but there is a small decrease in the accuracy when comparing the 6p elements. This could be a result of the WTBS generating function not being able to accurately describe the primary and secondary relativistic effects with only four different parameters. Improvements could be made by using two different sets of WTBS parameters. One of them would be optimized for the s and p spaces while the other would be optimized for the d and f spaces. The reasoning for why this would be a better idea is that the s and p spinors are affected the *primary* relativistic effect, and the d and f spinors are affected by the *secondary* relativistic effect. Because of this, it would be expected that using only one set of WTBS parameters would not be able to accuratly account for these two different affects.

It can also be seen Table 3.4 that the cudaDFRATOM basis sets are all larger than Dyall's basis sets. This is again a result of only using one set of four WTBS parameters, while Dyall

Calculated Energy ^{a}	Calculated Energy ^{b}	Total basis functions ^{a}	Total basis functions ^{b}
-7786.771	-7786.771	113	105
-8135.644	-8135.644	112	104
-15088.785	-15088.784	158	129
-15616.630	-15616.628	156	129
-16156.184	-16156.183	154	129
-16707.619	-16707.617	154	129
-17271.081	-17271.080	154	129
-17846.787	-17846.786	154	129
-18434.873	-18434.872	156	129
-19035.525	-19035.526	156	129
-19648.895	-19648.893	156	129
-20274.849	-20274.850	158	134
-20913.713	-20913.714	152	134
-21565.705	-21565.706	156	134
-22231.012	-22231.013	152	134
-22909.806	-22909.807	154	134
-23602.103	-23602.104	151	134
	Calculated Energy ^{a} -7786.771 -8135.644 -15088.785 -15616.630 -16156.184 -16707.619 -17271.081 -17846.787 -18434.873 -19035.525 -19648.895 -20274.849 -20913.713 -21565.705 -22231.012 -22909.806 -23602.103	Calculated EnergyaCalculated Energyb -7786.771 -7786.771 -8135.644 -8135.644 -15088.785 -15088.784 -15616.630 -15616.628 -16156.184 -16156.183 -16707.619 -16707.617 -17271.081 -17271.080 -17846.787 -17846.786 -18434.873 -18434.872 -19035.525 -19035.526 -19648.895 -19648.893 -20274.849 -20274.850 -20913.713 -20913.714 -21565.705 -21565.706 -2231.012 -2231.013 -23602.103 -23602.104	Calculated EnergyaCalculated EnergybTotal basis functionsa-7786.771-7786.771113-8135.644-8135.644112-15088.785-15088.784158-15016.630-15616.628156-16156.184-16156.183154-16707.619-16707.617154-17271.081-17271.080154-17846.787-17846.786154-18434.873-18434.872156-19035.525-19035.526156-19648.895-19648.893156-20274.849-20274.850158-20913.713-20913.714152-21565.705-21565.706156-22231.012-22231.013152-22909.806-22909.807154-23602.103-23602.104151

Table 3.4: Comparison of basis sets produced by cudaDFRATOM and Dyall's triple-zeta basis sets. The basis sets for the 6s[41], 6p[42], and 5d[43] elements are shown. The 4f elements were calculated with a different electron configuration, so they are omitted.

^acudaDFRATOM basis sets

^bDyalls basis sets

optimized each exponent individually. Therefore, he was able to achieve a high accuracy while using fewer basis functions. The above mentioned fix for improving accuracy in the 6p elements should also reduce the size of the basis sets so that they are more comparable in size to Dyall's.

Figures 3.2, 3.3, and 3.4 show the trends of various non-relativistic parameters with respect to nuclear charge. In Figure 3.2, we can see that there is an interesting pattern where the exponent of the most diffuse function becomes larger as we move right across a row. It is also interesting to note that the rate at which the exponent increases changes when going from one block of that row to the next. The trend roughly follows what we expect from periodic trends of atomic size: atoms get larger by going left on the table. The trend of atoms getting larger when moving down the periodic table is mostly obeyed, however there are exceptions. For instance, the 4d elements have smaller values of α than the 5d elements.

In Figure 3.3 shows that β generally decreases as nuclear charge increases. As β is involved in controlling the growth of the exponents, this indicates that the basis sets are getting more diffuse as the nuclear charge increases.

Finally 3.4 shows the values of δ and γ with respect to nuclear charge. There are no clear



Figure 3.2: Scatter plot of the α parameter vs. nuclear charge. Regions of the plot are shaded based on periodic table block regions. The s block is green, the p block is blue, the d block is red and the f block is yellow. There is a distinct pattern where the value of α increases along a row until a noble gas is reached. Also note how the rate of the increase changes at periodic table block boundaries.

trends in these parameters, but they are shown for completeness.

As for the relativistic basis sets, we can see from Figure 3.5 that the trend in α from the non-relativistic basis sets mostly holds, however there is a slight change in the trend starting at thallium. There is a substantial drop in the value of α when changing from the d to the p block in the relativistic basis sets which is not seen in the non-relativistic sets. We can also see that the change in α for the relativistic basis sets is much larger going through the d block than the change for the non-relativistic basis sets. As for the other WTBS parameters, the trends in the relativistic basis sets are mostly consistent with their non-relativistic counterparts. Figures for the remaining parameters are given in Figures 3.6 and 3.7.



Figure 3.3: Scatter plot of the β parameter vs. nuclear charge. Regions of the plot are shaded based on periodic table block regions. The s block is green, the p block is blue, the d block is red and the f block is yellow. There is a general trend of the value of β to decrease as the nuclear charge grows larger.



Figure 3.4: Scatter plots of the δ and γ parameters. Regions of the plot are shaded based on periodic table block regions. The s block is green, the p block is blue, the d block is red and the f block is yellow. There are no clear trends with respect to the nuclear charge.



Figure 3.5: Scatter plot of the relativistic and non-relativistic α parameters vs. nuclear charge. Regions of the plot are shaded based on periodic table block regions. The s block is green, the p block is blue, the d block is red and the f block is yellow.



Figure 3.6: Scatter plot of the relativistic and non-relativistic β parameters vs. nuclear charge. Regions of the plot are shaded based on periodic table block regions. The s block is green, the p block is blue, the d block is red and the f block is yellow.



Figure 3.7: Scatter plot of the relativistic and non-relativistic δ and γ parameters. Regions of the plot are shaded based on periodic table block regions. The s block is green, the p block is blue, the d block is red and the f block is yellow.

Chapter 4

Conclusions and Future Work

In this thesis I have illustrated how even small problems in computational quantum chemistry can benefit from parallel computation. I have done this both in the internal sense, where I rewrote the DFRATOM program to calculate the electronic structure of atoms on GPUs, and in the external sense, where I designed an algorithm that very effectively optimizes basis sets. This chapter will be broken up into two sections: the first which covers the rewriting of DFRATOM into cudaDFRATOM, and the second one which summarizes the results of basis set optimization using cudaDFRATOM and rwtbs.

4.1 cudaDFRATOM

By harnessing the power of GPUs, I was able get the cudaDFRATOM program to accelerate the biggest bottleneck of these calculations, the evaluation of the two-electron integrals, by almost a factor of 20. This changes the bottleneck to be the matrix operations required in SCF. As a result, the total speedup is only about 2-4 times faster than the original DFRATOM program. While this is not as much of an increase as we originally hoped, it is still a very big improvement on the original program.

It is also worth pointing out that as the problems get larger, the speedup gets larger as well. This indicates that the algorithms written for this program could potentially work even better on even larger problems such as molecules. Modifications required to make the algorithms work on molecules are as follows.

One could implement direct SCF. As the amount of two-electron integrals grows, it becomes impractical to try and store them all in memory. Instead, in the direct SCF algorithm, the integrals are calculated and consumed as needed. The current program has the following flow: the threads are mapped to all the integrals, all the integrals are calculated and stored in memory, and then all the integrals are used to form the \mathbf{P} and \mathbf{Q} matrices. If we wish to reuse as much of the code I've written as possible, the direct SCF implementation would work as follows. First we would map the threads to a chunk of the integrals, then we could calculate only that chunk, and then we would build up only the elements of the \mathbf{P} and \mathbf{Q} that use those integrals. Now, we no longer need these integrals, so we can throw them away and start the calculation of a new chunk. We would then loop over these steps until the the \mathbf{P} and \mathbf{Q} matrices have been completely calculated. The mapping takes very little time to calculate, so the fact that we are calling it so many times would have relatively little impact on performance.

One could also add some prescreening of the integrals to determine a rough estimate of their order of magnitude. If a particular integral is very close to zero, the effect it has on the calculation is relatively negligible. Therefore we could skip the calculation of this integral, and there would be almost no impact on the accuracy of the calculation. Due to how GPUs perform the calculations in warps, we would need to presort the integrals so that the ones that are likely to be close to zero are grouped together in order to maximize the returns of this procedure.

One would also need to alter the mapping algorithm so that it can handle calculations of different point groups. Atoms have spherical symmetry, meaning we can eliminate the need to calculate a lot of the integrals because many of them will be symmetrically the same. But this would not be the case in systems that have no symmetry, so we would need to change the mapping accordingly. This would actually be very simple to change, as we would just need to write nearly identical code for each symmetry that we would want to support.

One final comment regarding cudaDFRATOM is the algorithm to form the \mathbf{P} and \mathbf{Q} matrices. I am still not completely satisfied with the current state of this part of the code. It is quite complicated and inelegant. It would seem to me that there should be a better way of performing this calculation, but so far I have been unable to improve upon the version that appears in this thesis. One possible approach would be to break up the calculation of the matrices into two different subroutines: one that calculates \mathbf{P} and one that calculates \mathbf{Q} . The calculation of \mathbf{P} can be reformed into a simple matrix multiplication problem, but \mathbf{Q} requires many conditional statements as a result of having to deal with the math of open shells. I did not try this as I believed the main bottleneck was reading the two-electron integrals. Therefore, I only wanted to have to read them once to reduce the amount of global memory reads as possible. But it might be the case that specialized code for each matrix could outperform generalized code for both.

4.2 Basis Set Optimization

This thesis also covered the optimization of new basis sets. I used a novel algorithm that almost entirely eliminates the need for human involvement in the optimization process. It produces useful accurate basis sets, that are practically guarantied to be as small as possible. I have optimized non-relativistic basis sets for the elements helium through radon. I have also optimized relativistic basis sets for the elements caesium through radon. Future work in the area would be the optimization of relativistic basis sets for the rest of the periodic table. Care must be taken when optimizing sets for the seventh row elements, because the assumption made for kinetic balancing begins to break down there. As a result, early attempts to optimize basis sets for these elements have proven to be prone to prolapsing. As a result, the method of automating the optimization process should be used with caution in this range, as the results it produces may erroneously appear to be successful.

Further work that could be done includes modifications to the cudaDFRATOM program to support basis sets other than WTBS, and also to include other optimization algorithms than **newuoa**, which might be less prone to generating prolapsing basis sets. cudaDFRATOM also includes the option to optimize a different set of ζ s for different groups of spinor symmetries. Therefore, it might be best to try and optimize basis sets that have grouped the s and p type spinors into one group and the d and f type spinors in another. The logic of this is that relativity has different effects on these two groups, so it might be best to try and separate the two so that each gets its own set of specialized basis functions.

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Appendix A

cudaDFRATOM Input and Output files

This appendix shows cudaDFRATOM input files for a few common calculations. The output files are also given.

A.1 Single Point Energy with predefined WTBS parameters

This input file will perform a calculation on lead using predefined well-tempered basis set (WTBS) parameters. It uses the "autogen" option to automatically generate electron configurations.



Listing A.1: Input file for calculating the single point energy of Pb.

1	&CONTRL
2	JOBTYPE = energy,
3	C = 137.0359997600000
4	/
5	&NUC
6	ZNUC = 82.000000000000,
7	NUCMDL = 3,
8	RNUC = 0.0000000000000,
9	ALPHA = 137688400.8100000
0	/
.1	&BAS
2	NSYM = 7,
.3	BASTYPE = wtbs ,
.4	NGROUP = 1
.5	/
.6	&WTBS
7	WTBSPARA = 3.543348300000002E-002,
.8	1.83990500000000 ,
.9	4.486704200000000 ,
20	2.004835300000000 ,
21	NBS = 35,
22	30,
3	30,
:4	25,
10	25,
20	20,
00	20, CTAPT - 1
0	1 Jiniti – 1,
4.1	1,

30		1,					
31		1,					
32		1,					
34		1,					
35	GROUPS =	1,					
36		1,					
38		1,					
39		1,					
40		1,					
41 42	/	1					
43	&ECONFIG						
44	NCLOSE =	6,					
45 46		4,					
47		3,					
48		3,					
49		1,					
51	NOPEN =	0,					
52		1,					
53		1,					
55		0,					
56		0,					
57	PPPPPI -	0,					
59	AUTOGEN = T,	2,					
60	NCONF =	3					
61	/						
62	nconf = 3	2 00 0 00 0	00 0 00 0 00				
64	2 0.00 1.00	1.00 0.00 0	.00 0.00 0.00				
65	3 0.00 2.00	0.00 0.00 0	.00 0.00 0.00				
66	&SCF	FO					
68	IXTRP =	1,					
69	DFCTR = 0.300	000000000000000000000000000000000000000	,				
70	THDLL = 1.000	00000000000000000000000000000000000000	-005,				
72	THDSL = 9.995 THDSS = 1.000	0000000000000001E	-009				
73	/						
74	31560						
76 76	82680						
77	82680						
78	221424960		_				
80	Calculating one	e electron integ	grais				
81	Calculating gue	ess	51415				
82	Starting SCF						
83	SCF converged a	at iteration 21	Final energy =	-20913.7132	1671859		
85							
86		1S+	2S+	3S+	4S+	5S+	6S+
87		-3.2558910E+03	-5.8788484E+02	-1.4375419E+02	-3.3985791E+01	-6.1449434E+00	-5.6643943E-01
89							
90	3.5433483E-02	-1.9140257E-07	-9.7159398E-06	8.4857239E-05	2.1986574E-04	5.1415800E-04	2.0636937E-02
91	6.5194589E-02 1 1995578E-01	8.2570189E-07	4.1921119E-05	-3.6562370E-04 8 7018398E-04	-9.4709963E-04 2.2414603E-03	-2.1895500E-03	1.7096292E-01 4.6563303E-01
93	2.2073350E-01	3.5996723E-06	1.8260591E-04	-1.5762467E-03	-4.0630949E-03	-9.8724076E-03	4.9206077E-01
94	4.0626020E-01	-5.6936298E-06	-2.8865907E-04	2.4671919E-03	6.4082992E-03	-1.1737844E-02	1.8824719E-01
95 96	1.3783189F+00	8.3491287E-06	4.2257668E-04 -5.8146938F-04	-3.5241493E-03 4.8783856F-03	-8.9348378E-03	-2.9905373E-01	-3.0010508E-01
97	2.5427420E+00	1.5670362E-05	7.9374845E-04	-6.0504748E-03	2.7343372E-02	-5.2239957E-01	-2.8601945E-01
98	4.6995778E+00	-1.9958101E-05	-1.0286165E-03	6.5909755E-03	5.2434329E-01	7.2696910E-01	3.0687539E-01
99	8.7095624E+00	1.9050301E-05	1.1054521E-03	-2.3451833E-02	9.3510165E-01	8.5987922E-01	3.3842577E-01
101	3.0302910E+01	2.8420699E-05	3.7197373E-03	-8.1531809E-01	-1.0354558E+00	-5.7885493E-01	-2.0220940E-01
102	5.7068236E+01	7.7841668E-05	8.1191015E-02	-3.4478787E-01	-3.3138799E-01	-1.7960886E-01	-6.2968065E-02
103	1.0845021E+02	-1.7007069E-04	4.1109997E-01	4.9103230E-01	3.2296539E-01	1.5765479E-01	5.4052594E-02
$104 \\ 105$	4.0651542E+02	-2.9589527E-03	1.5500969E-01	4.6725787E-01 1.2163377E-01	6.9594624E-01	3.2609524E-02	4.3346064E-02
106	8.0667635E+02	-2.0848170E-01	-1.1977939E-01	-6.2191906E-02	-3.2239372E-02	-1.4726348E-02	-4.9831695E-03
107	1.6348107E+03	-2.9189696E-01	-1.6951366E-01	-8.7418119E-02	-4.4770915E-02	-2.0115505E-02	-6.7655030E-03
108	3.3969005E+03 7.2674336E+03	-2.4399046E-01 -1.5514532E-01	-1.23/4164E-01 -7.1929749E-02	-0.2334097E-02 -3.5560267E-02	-3.1043346E-02 -1.8046013E-02	-1.4364272E-02 -8.1052706E-03	-4.0398193E-03 -2.7270821E-03
110	1.6080864E+04	-8.5723247E-02	-3.7776777E-02	-1.8531501E-02	-9.3982955E-03	-4.2280724E-03	-1.4235773E-03
111	3.6974132E+04	-4.4254206E-02	-1.8890041E-02	-9.2074939E-03	-4.6580915E-03	-2.0916796E-03	-7.0381814E-04
112 113	8.8762050E+04 2.2355921F+05	-2.2211543E-02	-9.2756569E-03	-4.5077689E-03	-2.2802569E-03	-1.0247971E-03	-3.4495102E-04
114	5.9356339E+05	-5.4653284E-03	-2.2126683E-03	-1.0697906E-03	-5.4040349E-04	-2.4274024E-04	-8.1695794E-05
115	1.6690414E+06	-2.6711743E-03	-1.0700322E-03	-5.1634550E-04	-2.6065392E-04	-1.1702741E-04	-3.9380312E-05
$116 \\ 117$	4.9925105E+06	-1.2803414E-03	-5.0897019E-04	-2.4533622E-04	-1.2383272E-04	-5.5608079E-05	-1.8713930E-05
118	5.4660323E+07	-2.1789453E-04	-8.5878190E-05	-4.1336406E-05	-2.0856799E-05	-9.3648388E-06	-3.1514882E-06
119	2.0153596E+08	-2.1829984E-05	-8.5856049E-06	-4.1303396E-06	-2.0833500E-06	-9.3511877E-07	-3.1465061E-07
$120 \\ 121$	8.0207663E+08	1.5047170E-06	5.9151312E-07	2.8444110E-07	1.4340856E-07	6.4331467E-08	2.1641631E-08

100							
122	1.6143/50E+10	3.5734594E-08	1.4045396E-08	6.7527666E-09	3.4039038E-09	1.5265427E-09	5.1348999E-10
120	0.1990099E+10	-5.0509070E-09	-1.9675952E-09	-9.0009020E-10	-4.0100400E 11	-2.1001720E-10	-7.2002291E-11
124	4.55291406+11	5.//2/625E-10	2.2009040E-10	1.0906642E-10	5.490/090E-11	2.40595406-11	0.294/901E-12
125							
126							
127	3.5433483E-02	1.6954819E-09	-1.9755659E-08	1.0517252E-07	2.5786097E-07	6.0705258E-07	2.4548192E-05
128	6.5194589E-02	-6.1192070E-09	9.9944811E-08	-6.0718398E-07	-1.5143279E-06	-3.5153647E-06	2.7587966E-04
129	1.1995578E-01	1.2288718E-08	-2.9311326E-07	1.9454770E-06	4.8761399E-06	1.0747339E-05	1.0191707E-03
130	2.2073350E-01	-1.8377497E-08	6.7468779E-07	-4.7570165E-06	-1.2013960E-05	-2.9243701E-05	1.4610285E-03
131	4.0626020E-01	2.2094317E-08	-1.3755421E-06	1.0067995E-05	2.5740826E-05	-4.7401652E-05	7.5820245E-04
132	7.4802875E-01	-1.9732962E-08	2.6328827E-06	-1.9470061E-05	-4.8740114E-05	-1.6346171E-03	-1.6403132E-03
133	1.3783189E+00	7.0802976E-09	-4.7913481E-06	3.6517250E-05	1.1190759E-04	-5.7997109E-03	-3.7872066E-03
134	2.5427420E+00	3.3353393E-08	8.6948262E-06	-6.1451021E-05	2.7604343E-04	-5.2632551E-03	-2.8813285E-03
135	4.6995778E+00	-1.0558631E-07	-1.5093361E-05	9.0963356E-05	7.1885186E-03	9.9617188E-03	4.2051363E-03
136	8.7095624E+00	1.2906609E-07	2.2027770E-05	-4.3912334E-04	1.7443639E-02	1.6029779E-02	6.3081111E-03
137	1.6203217E+01	-3.6214254E-07	-3.8443478E-05	-6.1234284E-03	-2.9533854E-03	-1.4537621E-03	-5.7043669E-04
138	3.0302910E+01	5.2836853E-07	1.3285756E-04	-2.8417938E-02	-3.6003287E-02	-2.0119705E-02	-7.0279292E-03
139	5.7068236E+01	4.6114972E-06	3.9263140E-03	-1.6339710E-02	-1.5654581E-02	-8.4797945E-03	-2.9727261E-03
140	1.0845021E+02	-1.2950972E-05	2.7337032E-02	3.2407503E-02	2.1295257E-02	1.0391632E-02	3.5625331E-03
141	2.0847323E+02	-2.9073865E-04	4.6496978E-02	4.2189645E-02	2.4898158E-02	1.1543726E-02	3.9023181E-03
142	4.0651542E+02	-8.0613553E-03	1.9021333E-02	1.4724956E-02	8.4033363E-03	3.9370652E-03	1.3390133E-03
143	8.0667635E+02	-3.9844448E-02	-2.1952178E-02	-1.1434990E-02	-5.9321659E-03	-2.7091031E-03	-9.1660186E-04
144	1.6348107E+03	-7.7242278E-02	-4.2059759E-02	-2.1528276E-02	-1.1006504E-02	-4.9428729E-03	-1.6622820E-03
145	3.3969005E+03	-8.8701783E-02	-4.2001749E-02	-2.0959345E-02	-1.0683736E-02	-4.8172258E-03	-1.6229926E-03
146	7.2674336E+03	-7.6482772E-02	-3.3116809E-02	-1.6206858E-02	-8.2039085E-03	-3.6819580E-03	-1.2386094E-03
147	1.6080864E+04	-5.6100232E-02	-2.3179626E-02	-1.1261204E-02	-5.6984512E-03	-2.5626001E-03	-8.6278680E-04
148	3.6974132E+04	-3.7347045E-02	-1.5052553E-02	-7.2708423E-03	-3.6698025E-03	-1.6466392E-03	-5.5396552E-04
149	8.8762050E+04	-2.3278150E-02	-9.2698061E-03	-4.4718637E-03	-2.2583779E-03	-1.0147581E-03	-3.4157455E-04
150	2.2355921E+05	-1.3784938E-02	-5.4532697E-03	-2.6256301E-03	-1.3243959E-03	-5.9430475E-04	-1.9995104E-04
151	5.9356339E+05	-7.7805110E-03	-3.0685330E-03	-1.4775435E-03	-7.4574987E-04	-3.3497969E-04	-1.1274508E-04
152	1.6690414E+06	-4.1729867E-03	-1.6425066E-03	-7.9020592E-04	-3.9854800E-04	-1.7886230E-04	-6.0180408E-05
153	4.9925105E+06	-2.0861996E-03	-8.2044252E-04	-3.9483492E-04	-1.9924164E-04	-8.9483516E-05	-3.0116278E-05
154	1.5952595E+07	-9.3209819E-04	-3.6627633E-04	-1.7617169E-04	-8.8851596E-05	-3.9876899E-05	-1.3417320E-05
155	5.4660323E+07	-2.8134459E-04	-1.1055138E-04	-5.3198526E-05	-2.6846343E-05	-1.2058514E-05	-4.0585399E-06
156	2.0153596E+08	-5.0398556E-06	-1.9824128E-06	-9.4788639E-07	-4.7454755E-07	-2.1080489E-07	-7.0655962E-08
157	8.0207663E+08	-9.6484793E-07	-3.7958549E-07	-1.8491005E-07	-9.4673401E-08	-4.3358342E-08	-1.4697821E-08
158	3.4548830E+09	4.2903511E-07	1.6878873E-07	8.2035379E-08	4.1888247E-08	1.9114999E-08	6.4712118E-09
159	1.6143750E+10	-1.5185021E-07	-5.9740539E-08	-2.9026287E-08	-1.4815664E-08	-6.7575308E-09	-2.2872876E-09
160	8.1990099E+10	4.8899010E-08	1.9237777E-08	9.3465918E-09	4.7703943E-09	2.1756194E-09	7.3637952E-10
161	4.5329140E+11	-1.3146726E-08	-5.1721694E-09	-2.5128521E-09	-1.2825163E-09	-5.8490432E-10	-1.9797080E-10
162							
163		0.0	0.0	15	50	CD	
164		2P-	1 2000200E 02	4P-	5P-	0.7507060E 01	
166		-5.6346/04E+02	-1.3260392E+02	-2.92110106+01	-4.4404008E+00	-2.7507200E-01	
167							
T () (
168	3.5433483E-02	-2.1110836E-06	3.3329049E-05	8.2318337E-05	-2.3099532E-04	-9.5114313E-02	
168 169	3.5433483E-02 6.5194589E-02	-2.1110836E-06	3.3329049E-05	8.2318337E-05	-2.3099532E-04	-9.5114313E-02	
168 169 170	3.5433483E-02 6.5194589E-02 1.1995578E-01	-2.1110836E-06 8.2038732E-06 -1.8429299E-05	3.3329049E-05 -1.2966616E-04 2.8944290E-04	8.2318337E-05 -3.2228822E-04 7.0702895E-04	-2.3099532E-04 1.1078969E-03 -1.5754355E-03	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01	
168 169 170 171	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04	8.2318337E-05 -3.2228822E-04 7.0702895E-04 -1.2533334E-03	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 6.4782033E-03	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01	
168 169 170 171 172	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04	8.2318337E-05 -3.2228822E-04 7.0702895E-04 -1.2533334E-03 1.8997745E-03	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 6.4782033E-03 2.6096020E-02	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01	
168 169 170 171 172 173	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 7.4802875E-01	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03	8.2318337E-05 -3.2228822E-04 7.0702895E-04 -1.2533334E-03 1.8997745E-03 -2.6453479E-03	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 6.4782033E-03 2.6096020E-02 2.1315146E-01	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02	
168 169 170 171 172 173 174	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 7.4802875E-01 1.3783189E+00	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0242435E-04	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 1.5950138E-03	8.2318337E-05 -3.2228822E-04 7.0702895E-04 -1.2533334E-03 1.8997745E-03 -2.6453479E-03 5.1813384E-03	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 6.4782033E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01	
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$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.6026020E-01 1.3783139E-00 2.5427420E+00 4.6995778E+00 8.7095624E+00 1.6203217E+01 5.7066236E+01 1.0845021E+02 2.0847323E+02 4.0651542E+02 8.0667635E+02 1.6348107E+03 3.3966005E+03 7.2674336E+03	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0242435E-04 -1.9939967E-04 1.8953650E-04 9.7479204E-04 2.2896984E-02 1.5476535E-01 3.1765576E-01 3.1357302E-01 2.0254176E-01 5.0059648E-02 2.369416E-02 2.369416E-02	3.3329049E-05 -1.2964616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 1.1223456E-03 1.5950138E-03 -2.0117491E-03 2.2268120E-03 -9.3713975E-03 -9.7628883E-02 -4.2695288E-01 -1.0565728E-01 1.6311570E-01 1.8279811E-01 1.837400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 2.6435568E-02	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 5.1813384E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 6.2243748E-01 6.2243748E-01 -3.0935771E-01 -4.003696E-01 -9.4601050E-02 7.9749840E-02 9.520998E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 3.018	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 6.4782033E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 -4.849021E-01 -4.849021E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 4.4583201E-02 -3.3447982E-02 -4.0980859E-02 -2.4840415E-02 -2.4840415E-02 -1.246354E-02 -5.6918307E-03 -2.6582428E-03 -1.286754E-02 -1.286754E-02 -1.286754E-03 -2.6582428E-03 -1.286754E-03 -2.6582428E-03 -2.5582428E-03 -2.5582428E-03 -2.5582428E-03 -2.5582428E-03 -2.5582428E-03 -2.5582428E-03 -2.5582428E-03 -2.5582428E-03 -2.558248	-9,5114313E-02 -2,4887441E-01 -3,8418187E-01 -3,1103172E-01 -1,4702572E-01 7,3403494E-02 2,0051539E-01 1.8040757E-01 -2,2131882E-02 -1,3477866E-01 -6,6197533E-02 3,6084562E-02 5,1750801E-02 -8,8056305E-03 -1,0840501E-02 -6,513532E-03 -1,5028703E-03 -1,5028703E-03 -7,0213261E-04 -3,3918314E-04	
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$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 7.4802875E-01 1.3783189E+00 2.5427420E+00 4.6995778E+00 8.7095624E+00 1.6203217E-01 3.0302910E+01 5.7068236E+01 1.0845021E+02 2.0847332E+02 4.0651542E+02 2.6067635E+02 1.6348107E+03 3.3969005E+03 3.3969005E+04 3.60864E+04 3.6974132E+04 4.87605E+04	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0224236E-04 1.4757652E-04 1.4757652E-04 3.7221586E-04 9.7479204E-04 2.2896984E-02 1.547653E-01 3.1765576E-01 3.1357302E-01 1.0554176E-01 5.0059164E-02 2.3694166E-02 1.1638547E-02 5.9982431E-03 3.19322F-03 1.0325F-03	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 1.5950138E-03 -2.0117491E-03 2.2268120E-03 9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -1.0565728E-01 1.6311570E-01 1.834700E-01 5.7122173E-02 2.6435568E-02 2.6435568E-02 1.2341259E-02 6.0023349E-03 3.0784422E-03	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 -2.6453479E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 6.2243748E-01 3.4575529E-01 -3.0935771E-01 -4.003696E-02 9.4601050E-02 7.9749840E-02 9.58154906E-02 2.9134598E-02 1.3361681E-02 2.316645E-03 3.0182407E-03 1.5480368E-03 8.1963068E-03	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -4.6368432E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 1.44583201E-02 -3.3447982E-02 -4.0980859E-02 -2.4840415E-02 -1.2463954E-02 -5.6918307E-03 -2.6582428E-03 -1.2847058E-03 -6.5951230E-04	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 -1.3477866E-01 -6.6197533E-02 3.6084562E-02 5.1750801E-02 -1.1943673E-02 -8.8056305E-03 -1.0840501E-02 -6.5631352E-03 -3.2936776E-03 -3.2936776E-03 -1.0212703E-03 -7.02128703E-04 -3.3918314E-04 -1.7415861E-04 -1.7415861E-04 -2.2124704E-05 -1.5615202	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191 \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.6026020E-01 1.3783189E-00 2.5427420E+00 4.6995778E+00 8.7095624E+00 1.6203217E+01 5.7066236E+01 1.0845021E+02 2.0847328E+02 4.0651542E+02 8.0667635E+02 1.6348107E+03 3.3966005E+03 7.2674336E+03 1.6080864E+04 8.6974132E+04 8.8762050E+04	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0242435E-04 1.4757652E-04 1.9939967E-04 3.7221586E-04 9.7479204E-04 2.2896984E-02 1.5476535E-01 3.1765576E-01 3.1765576E-01 3.1357302E-01 1.0544176E-01 2.0254912E-01 1.05844176E-01 5.0059648E-02 2.3694166E-02 2.3694166E-02 2.369416E-03 3.193122E-03 3.193122E-03 3.1733122E-03	3.3329049E-05 -1.2964616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 1.1223456E-03 1.5950138E-03 -2.0117491E-03 2.2268120E-03 -9.3713975E-03 -9.7628883E-02 -4.2695288E-01 -1.0565728E-01 1.6311570E-01 1.8279811E-01 1.8379811E-01 1.837568E-02 2.6435568E-02 2.6435568E-02 1.2341259E-02 3.0784422E-03 3.0784422E-03 1.6331902E-03	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 5.1813384E-03 5.1813384E-03 5.1813384E-02 2.666845E-02 2.666845E-02 2.6664648E-01 6.2243748E-01 -3.0935771E-01 -4.003696E-02 9.5209988E-02 5.8154906E-02 2.9134598E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 8.1995336E-04 4.4204912F-04	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 6.4782033E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 -4.8490218E-01 -1.0409201E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 1.3640741E-02 -3.3447982E-02 -2.4840415E-02 -1.2463954E-02 -5.6918307E-03 -2.6582428E-03 -1.2847058E-03 -1.284	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 -1.3477866E-01 3.6084562E-02 5.1750801E-02 -8.8056305E-03 -1.0940501E-02 -8.8056305E-03 -1.5028703E-03 -3.2936776E-03 -1.5028703E-03 -3.3918314E-04 -1.7415861E-04 -9.2142104E-05 -4.960948E-05	
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$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 193\end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3733189E-00 2.5427420E+00 4.6995778E+00 1.6203217E+01 3.0302910E+01 5.7066236E+01 1.6845021E+02 2.0847332E+02 1.6348107E+03 3.3969005E+03 7.2674336E+03 1.6080864E+04 3.6974132E+04 8.8762050E+04 2.355921E+05 5.9356339E+05 5.9356339E+05	-2.1110836E-06 8.2038732E-06 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0224235E-04 -1.933967E-04 1.8953650E-04 9.7479204E-04 2.2896984E-02 1.5476535E-01 3.1765576E-01 3.1765576E-01 3.1765576E-01 3.1765576E-01 1.0544176E-01 1.059648E-02 2.3694166E-02 1.1638547E-02 5.9982431E-03 3.193125E-03 1.7236138E-03 9.1977675E-04 4.7923138E-03	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 1.5950138E-03 -2.0117491E-03 2.2268120E-03 9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -1.0565728E-01 1.6311570E-01 1.1347400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 6.0023349E-03 3.0784422E-03 3.0784422E-03 3.6331902E-03 8.8035369E-04 4.6933992E-04	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 -1.6453479E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 6.2243748E-01 3.4575529E-01 -4.0033696E-01 -9.4601050E-02 9.520998E-02 5.8154906E-02 2.9134598E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 3.0182407E-03 1.5480068E-03 1.5480068E-04 4.4204912E-04 2.3584732E-04 1.2268495E-04	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -1.0409201E-01 1.9231613E-01 4.4538201E-02 -3.3447982E-02 -2.3504320E-01 1.9231613E-02 -4.0980859E-02 -2.4840415E-02 -1.2463954E-02 -2.658242E-03 -1.2847058E-03 -1.2847058E-03 -3.4899562E-04 -1.8822394E-04 -1.0026146E-04	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 1.3477866E-01 -6.6197533E-02 3.6084562E-02 5.1750801E-02 1.1943673E-02 -8.8056305E-03 -1.0840501E-02 -6.5613532E-03 -3.2936776E-03 -1.0528703E-03 -7.0213261E-04 -3.3918314E-04 -1.7415861E-04 -9.2142104E-05 -4.9699458E-05 -2.6471634E-05 -1.3792011E-05	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 194\end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 7.4802875E-01 1.3783189E+00 2.5427420E+00 4.6995778E+00 8.7095624E+00 1.6203217E-01 3.0302910E+01 5.7068236E+01 1.0845021E+02 2.0847323E+02 4.0651542E+02 2.0847332E+03 3.3969005E+03 3.3969005E+03 1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05 1.6690414E+06 4.9925105E+06	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0242435E-04 1.4757652E-04 1.8953650E-04 9.7479204E-04 2.2896984E-02 1.547653E-01 3.1765576E-01 3.1357302E-01 1.0544176E-01 5.0059648E-02 2.3694166E-02 1.1638547E-02 5.9982431E-03 3.1931225E-03 1.7236138E-03 9.1977675E-04 4.7923133E-04 2.3419075E-04	3.3329049E-05 -1.2966616E-04 2.8944290E-05 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 2.20117491E-03 2.20117491E-03 2.20117491E-03 9.3713975E-03 -9.762883E-02 -4.2695288E-01 -4.9060947E-01 -1.0565728E-01 1.6311570E-01 1.8279811E-01 1.1347400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 6.0023349E-03 3.0784422E-03 3.0784422E-03 3.8315369E-04 4.6933992E-04 4.6933992E-04 1.1943149E-04	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 -2.6453479E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 6.2243748E-01 3.4575529E-01 -3.0935771E-01 -4.003696E-02 9.4601050E-02 7.9749840E-02 9.4601050E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.549036E-04 4.4204912E-04 2.3554733E-04 1.9298985E-02 1.3554732E-05 .934273E	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -4.6368432E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 1.9231613E-01 -2.3504320E-02 -3.3447982E-02 -2.4840415E-02 -2.4840415E-02 -1.2463954E-02 -1.2463954E-03 -1.2847058E-03 -1.2847058E-03 -1.2847058E-04 -1.822394E-04 -1.822394E-04 -5.2235504E-05 -2.5511986E-05	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 -1.3477866E-01 -6.6197533E-02 3.6084562E-02 5.1750801E-02 -8.8056305E-03 -1.0840501E-02 -8.8056305E-03 -1.0840501E-02 -8.32936776E-03 -3.2936776E-03 -3.2936776E-03 -1.5213221E-04 -3.3918314E-04 -1.7415861E-04 -4.969458E-05 -2.6471634E-05 -1.3792011E-05 -6.735838E-06	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 188\\ 188\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3733189E-00 2.5427420E+00 1.6203217E+01 3.0302910E+01 5.7066236E+01 1.0845021E+02 2.0847323E+02 4.0651542E+02 8.0667635E+02 1.6348107E+03 3.3966005E+03 7.2674336E+03 1.6608084E+04 8.8762050E+04 8.8762050E+04 1.6592414E+06 4.9925105E+06 1.5652595E+07	-2.1110836E-06 8.2038732E-06 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.024233E-04 -1.939967E-04 1.8953650E-04 -3.7221586E-04 9.7479204E-04 2.2886884E-02 1.5476535E-01 3.157302E-01 2.0254912E-01 1.0544176E-01 5.0059648E-02 2.3694166E-02 2.3694166E-02 2.369416E-03 3.1931225E-03 3.1931225E-03 3.1931225E-04 4.7923133E-04 2.3419075E-04 1.0466575E-04	3.3329049E-05 -1.2964616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 1.1223456E-03 1.5950138E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -1.0565728E-01 1.6311570E-01 1.8279811E-01 1.1347400E-01 1.8279811E-01 1.3241258E-02 2.6435568E-02 1.2341258E-03 3.0784422E-03 3.035369E-04 4.6933992E-04 2.4346020E-04 1.1943149E-04 5.3372488E-05	8.2318337E-05 -3.2228622E-04 7.070295E-04 1.2533334E-03 1.8997745E-03 2.6453479E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 6.2243748E-01 3.4575529E-01 -3.0935771E-01 -4.0035671E-01 -9.4601050E-02 7.9749840E-02 7.9749840E-02 7.9749840E-02 2.9134598E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 8.1995336E-04 4.4204912E-04 2.3554723E-04 1.2269895E-04 5.9934572E-05 2.6785502E-05	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 6.4782033E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 -4.8490218E-01 -1.0409201E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 1.3640741E-01 1.9231613E-02 -3.3447982E-02 -4.0980859E-02 -2.4840415E-02 -1.2463954E-02 -5.6918307E-03 -2.5651230E-04 -3.4899562E-04 -1.822394E-04 -1.822394E-04 -1.8223504E-05 -2.5511986E-05 -1.1402544E-05	-9,5114313E-02 -2,4887441E-01 -3,8418187E-01 -3,103172E-01 -1,4702572E-01 7,3403494E-02 2,0051539E-01 1.8040757E-01 -2,2131882E-02 -1,3477866E-01 -6,6197538E-02 3,6084562E-02 5,1750801E-02 -8,8056305E-03 -1,0840501E-02 -8,8056305E-03 -1,028703E-03 -1,5028703E-03 -1,5028703E-03 -1,5028703E-03 -1,5028703E-03 -3,3918314E-04 -9,2142104E-05 -2,6471634E-05 -1,3792011E-05 -6,7358838E-06 -3,0106423E-06	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 188\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 196\\ 196\\ 196\\ 196\\ 196\\ 196\\ 196$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3783189E+00 2.5427420E+00 1.6203217E+01 3.0302910E+01 1.0845021E+02 2.0847332E+02 2.0847332E+02 4.0651542E+02 8.0667635E+02 1.6348107E+03 3.3369005E+03 7.2674336E+03 1.660864E+04 4.8762050E+04 2.2355921E+05 5.9356339E+05 1.6690414E+06 4.9925105E+06 5.9460332E+07 5.4660332E+07	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 1.0242435E-04 1.4757652E-04 -1.933967E-04 9.7479204E-04 9.7479204E-04 2.2856984E-02 1.5476535E-01 3.1357302E-01 2.0254912E-01 1.0544176E-01 2.0369416E-02 5.095648E-02 5.9982431E-03 3.1931225E-03 1.7236138E-03 9.1977675E-04 4.7923133E-04 2.3692464E-05	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 -2.0117491E-03 2.208120E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -1.0565728E-01 1.63219811E-01 1.1347400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 6.0023349E-03 3.0784422E-03 1.6331902E-04 4.6933992E-04 2.4446020E-04 1.1943149E-04 5.3372488E-05 1.5649976E-05	8.2318337E-05 -3.222822E-04 7.070285E-03 1.253334E-03 1.8997745E-03 -2.6453479E-03 2.1606845E-02 2.6654648E-01 3.4575529E-01 -3.0935771E-01 -9.4601050E-02 7.9749840E-02 9.5209986E-02 5.8154906E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 3.1954368E-04 4.4204912E-04 4.205985E-04 5.26785502E-04 5.26785502E-05 7.8534060E-06 85502E-05 855	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -1.0409201E-01 1.3640741E-01 1.9231613E-01 4.4583201E-02 -2.4840741E-01 1.9231613E-01 4.4583201E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-03 -2.5561230E-04 -3.4892562E-04 -1.822394E-04 -1.0026146E-04 -5.235504E-05 -1.1402544E-05 -3.3429305E-06	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 3.6084562E-02 5.1750801E-02 1.1943673E-02 -8.8056305E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-03 -1.3792011E-05 -2.6471634E-05 -3.0106423E-06 -3.8262848E-07	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 183\\ 184\\ 185\\ 186\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ 197\\ \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3783189E+00 2.5427420E+00 4.6995778E+00 1.6203217E+01 3.0302910E+01 1.0845021E+02 2.0847332E+02 4.0651542E+02 8.0667635E+02 1.6348107E+03 3.3969005E+03 7.2674336E+03 1.6080864E+04 8.8762050E+04 2.355921E+05 5.9356339E+05 1.6690414E+06 4.9925105E+06 1.5952555E+07 5.466032E+07 2.0153596E+08	-2.1110836E-06 8.2038732E-06 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.022423E-04 1.4757652E-04 -1.9339967E-04 2.2896984E-02 1.5476535E-01 3.1357302E-01 2.0254912E-01 1.0544176E-01 3.0559648E-02 2.3694166E-02 1.1638547E-02 5.9059648E-02 3.1931225E-03 1.7236138E-03 9.1977675E-04 4.792313E-04 2.3419075E-04 3.0692464E-05 8.6822796E-07	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 1.5950138E-03 -2.0117491E-03 2.2268120E-03 9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -1.665728E-01 1.6311570E-01 1.1347400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 6.0023349E-03 3.0784422E-03 3.0784422E-03 3.6331902E-03 8.8035369E-04 4.6933992E-04 4.6339392E-04 4.1943149E-04 5.372488E-05 1.5649976E-05 4.428491E-07	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 -1.6453479E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 3.4575529E-01 -3.0935771E-01 -4.0033696E-01 -9.4601050E-02 9.520998E-02 5.8154906E-02 2.9134598E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 3.0182407E-03 1.5480068E-03 3.0182407E-03 1.5480068E-04 4.4204912E-04 2.3554723E-04 4.2269895E-04 5.9934273E-05 2.6785502E-05 7.8534068E-07	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -1.0409201E-01 1.3640741E-01 1.9231613E-01 4.4538201E-02 -3.3447982E-02 -2.4840415E-02 -1.2463954E-02 -2.658242E-03 -1.2847058E-03 -1.2847058E-03 -1.2847058E-03 -3.4899562E-04 -1.8822394E-04 -1.8822394E-04 -1.0026146E-04 -2.5511986E-05 -2.5511986E-05 -3.3429305E-06 -9.4676609E-08	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 1.3477866E-01 -6.6197533E-02 3.6084562E-02 5.1750801E-02 1.1943673E-02 -8.8056305E-03 -1.0840501E-02 -6.5613532E-03 -1.0528703E-03 -1.0528703E-03 -1.5028703E-03 -1.3931314E-04 -1.7415861E-04 -2.49699458E-05 -2.6471634E-05 -1.3792011E-05 -1.3782011E-05 -3.106423E-06 -3.0106423E-06 -3.0106423E-06 -3.0106423E-06	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 183\\ 184\\ 185\\ 188\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ 198\\ \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.6026020E-01 1.3783189E-00 2.5427420E+00 4.6995778E+00 8.7095624E+00 1.6203217E+01 5.7066236E+01 1.0845021E+02 2.0847328E+02 4.0651542E+02 8.0667635E+02 1.6348107E+03 3.3969005E+03 7.2674336E+03 1.660864E+04 3.6974132E+04 8.762050E+04 2.355921E+05 5.9356339E+05 1.6690414E+06 4.9925105E+06 1.5952595E+07 5.4660332E+07 2.0153596E+08	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0242435E-04 1.4757652E-04 -1.939967E-04 9.7479204E-04 1.8953650E-04 -3.7221586E-01 3.1765576E-01 3.1357302E-01 1.0544176E-01 5.0059648E-02 2.3694166E-02 1.1638547E-02 5.9982431E-03 3.1931225E-03 1.7236138E-03 9.1977675E-04 4.7923133E-04 2.3419075E-04 1.0466575E-04 3.0692464E-05 8.6822796E-07	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 2.20117491E-03 2.2268120E-03 9.3713975E-03 -9.762883E-02 -4.2695288E-01 1.6365728E-01 1.6365728E-01 1.6371570E-01 1.334700E-01 5.7122173E-02 2.6435568E-02 1.6331902E-03 3.0784422E-03 3.633992E-04 4.6933992E-04 4.6933992E-04 4.53372488E-05 1.5649976E-05 4.4288491E-07	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 5.1813384E-03 2.4665445E-02 2.6654648E-01 6.2243748E-01 3.4575529E-01 -3.0935771E-01 -4.003696E-01 -9.4601050E-02 7.9749840E-02 9.5209988E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 8.1995336E-04 4.4204912E-04 2.3554733E-05 2.6785502E-05 7.8534060E-06 2.2234096E-07	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -4.6368432E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 1.9231613E-01 -2.3504320E-02 -3.3447982E-02 -4.0980859E-02 -2.4840415E-02 -2.4840415E-02 -1.2463954E-03 -1.2847058E-03 -1.2847058E-03 -1.2847058E-03 -1.2847058E-03 -2.5511380E-04 -1.822394E-04 -1.0226146E-04 -2.5511386E-05 -1.1402544E-05 -3.3429305E-06 -9.4676609E-08	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 -1.3477866E-01 -6.6197533E-02 3.6084562E-02 5.1750801E-02 -8.8056305E-03 -1.0840501E-02 -8.8056305E-03 -1.0840501E-02 -8.32936776E-03 -3.2936776E-03 -3.2936776E-03 -3.3918314E-04 -1.7415861E-04 -3.3918314E-04 -1.7415861E-04 -4.9699458E-05 -2.6471634E-05 -1.3792011E-05 -6.735838E-06 -3.0106423E-06 -8.8262848E-07 -2.4999155E-08	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 188\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ 198\\ 198\\ 199\\ 199$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3733189E-00 2.5427420E+00 1.6203217E+01 3.0302910E+01 5.7068236E+01 1.0845021E+02 2.0847323E+02 4.0651542E+02 8.0667635E+02 7.2674336E+03 7.2674336E+03 7.2674336E+03 7.2674336E+03 1.6600464E+04 8.8762050E+04 2.3355921E+05 5.356533E+05 1.6690414E+06 4.9925105E+06 1.5952556E+07 5.4660323E+07 2.0153596E+08	-2.1110836E-06 8.2038732E-06 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0242435E-04 -1.939967E-04 -3.7221586E-04 9.7479204E-02 1.5476535E-01 3.1765576E-04 2.2896984E-02 1.5476535E-01 3.1357302E-01 2.0254912E-01 1.0544176E-02 1.638547E-02 2.3694166E-02 2.3694166E-02 1.638547E-03 3.1931225E-03 3.1931225E-03 3.1931225E-03 1.7236138E-03 3.1931225E-03 1.7236138E-04 2.3419075E-04 4.7923133E-04 2.3419075E-04 3.0692464E-05 8.6822796E-07	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 1.1223456E-03 1.5950138E-03 -2.0117491E-03 9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -4.9060947E-01 -1.0565728E-01 1.6311570E-01 1.63219811E-01 1.3279811E-01 1.3279811E-01 1.3279811E-01 1.3279811E-01 3.0784422E-03 1.6331902E-03 8.8035369E-04 4.6933992E-04 2.3446020E-04 1.1943149E-04 5.3372488E-05 1.5649976E-05 4.4288491E-07	8.2318337E-05 -3.222822E-04 7.070285E-04 1.2533334E-03 1.8997745E-03 -2.6453479E-03 2.1606845E-02 2.6654648E-01 3.4575529E-01 -3.0935771E-01 -9.4601050E-02 7.9749840E-02 2.9134598E-02 2.9134598E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 3.0182407E-03 3.0182407E-03 3.15480068E-03 3.15480068E-03 3.15480068E-03 3.1526078E-04 1.2269895E-04 5.9334273E-04 1.2269895E-04 5.9334273E-05 7.8534060E-06 2.2234096E-07	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 4.8490218E-01 4.8490218E-01 -1.0409201E-01 1.3640741E-01 1.3640741E-01 1.9231613E-01 4.4583201E-02 -3.3447982E-02 -2.4840415E-02 -1.2463954E-02 -2.4840415E-02 -1.2463954E-03 -2.6582428E-03 -1.2847058E-03 -1.2847058E-03 -1.2847058E-04 -1.822394E-04 -1.8223504E-05 -2.5511986E-05 -3.3429305E-06 -9.4676609E-08	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 3.6084562E-02 3.6084562E-02 1.1943673E-02 -5.1758001E-02 1.0846501E-02 -6.5613532E-03 -3.2936776E-03 -3.2936776E-03 -1.5028703E-03 -7.0213261E-04 -3.3918314E-04 -9.2142104E-05 -4.9699458E-05 -1.3792011E-05 -6.7358838E-06 -8.8262848E-07 -2.4999155E-08	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ 198\\ 199\\ 200\\ 200\\ \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3783189E+00 2.5427420E+00 1.6203217E+01 3.0302910E+01 1.0845021E+02 2.0847332E+02 2.0847332E+02 4.0651542E+02 8.0667635E+02 1.6348107E+03 3.3369005E+03 7.2674336E+03 1.660864E+04 4.8762050E+04 2.2355921E+05 5.9356339E+05 1.6690414E+06 4.9925105E+06 5.5952595E+07 2.0153596E+08	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 1.022423E-04 1.4757652E-04 -1.933967E-04 9.7479204E-04 2.2856984E-02 1.5476535E-01 3.1765576E-01 3.1357302E-01 2.0254912E-01 1.0544176E-01 2.0369416E-02 2.369416E-02 5.9982431E-03 3.1931225E-03 1.7236138E-03 9.1977675E-04 4.7923133E-04 2.3692464E-05 8.6822796E-07 -8.5886264E-06	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 -2.0117491E-03 2.208120E-03 9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -1.0565728E-01 1.6311570E-01 1.6327841E-01 1.1347400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 6.0023349E-03 3.0784422E-03 1.6331902E-04 4.6933992E-04 2.4446020E-04 1.1543149E-04 4.53372488E-05 1.5649976E-05 4.4288491E-07 -3.8710980E-08	8.2318337E-05 -3.2228822E-04 7.070285E-03 1.2533334E-03 1.8997745E-03 2.6453479E-03 2.1606845E-02 2.6654648E-01 3.4575529E-01 -3.0935771E-01 -9.4601050E-02 7.9749840E-02 2.9134598E-02 5.8154906E-02 2.9134598E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 3.1954328E-04 4.4204912E-04 4.205985E-04 5.9934273E-05 2.6785502E-05 7.8534060E-07 -1.3229008E-06 -1.3229008E-06	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -1.0409201E-01 1.3640741E-01 1.9231613E-01 4.4583201E-02 -2.3504320E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-03 -2.5551230E-04 -3.4899562E-04 -1.822394E-04 -1.0026146E-04 -5.235504E-05 -2.5511986E-05 -1.1402544E-05 -3.3429305E-06 -9.4676609E-08 -1.4244408E-07 -2.52410E-07	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 3.6084562E-02 3.6084562E-02 5.1750801E-02 1.943673E-03 -6.5613532E-03 -1.5028703E-03 -1.5028703E-03 -1.5028703E-04 -2.6471634E-04 -2.6471634E-05 -2.6471634E-05 -2.6471634E-05 -2.6471634E-05 -2.6471634E-05 -2.6471634E-05 -3.0106423E-06 -3.0106423E-08 -3.24999155E-08 -1.4597307E-04 -1.4597307E-04	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ 198\\ 199\\ 200\\ 201\\ 200\\ 201\\ 201\\ 201\\ 201\\ 201$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3733189E+00 2.5427420E+00 4.6995778E+00 1.6203217E+01 3.0302910E+01 5.7066236E+01 1.6845021E+02 2.0847332E+02 2.0847332E+02 1.6348107E+03 3.3969005E+03 7.2674336E+03 1.6080864E+04 3.6974132E+04 4.8762050E+04 2.355921E+05 5.9356339E+05 5.9356339E+05 5.9356339E+05 1.6690414E+06 4.9925105E+06 1.595255E+07 5.4660323E+07 2.0153596E+08	-2.1110836E-06 8.2038732E-06 1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0224235E-04 1.9393967E-04 1.3953650E-04 9.7479204E-04 2.2896984E-02 1.5476535E-01 3.1765576E-01 3.1765576E-01 3.059648E-02 2.3694166E-02 1.638547E-02 5.9982431E-03 3.1931225E-03 1.7236138E-03 9.1977675E-04 4.7923133E-04 2.3419075E-04 3.0692464E-05 8.6822796E-07 -8.5886264E-06 4.8437004E-06	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 .2268120E-03 2.208120E-03 2.208120E-03 9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3762883E-02 -4.2695288E-01 1.6351570E-01 1.6351570E-01 1.6351570E-01 1.32470811E-01 1.347400E-01 5.7122173E-02 2.643568E-02 1.2341259-02 6.0023349E-03 3.0784422E-03 3.0784422E-03 3.6331902E-03 8.8035369E-04 4.53372488E-05 1.5649976E-05 1.5649976E-05 4.4288491E-07 -3.8710980E-08 -2.3081520E-07	8.2318337E-05 -3.2228822E-04 7.0702895E-04 1.253334E-03 1.8997745E-03 -2.6453479E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 6.2243748E-01 3.4575529E-01 -3.0935771E-01 -4.0033696E-01 -9.4601050E-02 9.520998E-02 5.8154906E-02 2.9134598E-02 1.3361681E-02 2.9134598E-02 1.3361681E-02 2.9134598E-02 1.3361681E-03 3.0182407E-03 1.5480068E-03 3.0182407E-03 1.5480068E-04 1.2269895E-04 5.934273E-05 2.6785502E-05 7.8534060E-06 2.2234096E-07 -1.3229008E-06 1.4609437E-07	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -4.6368432E-01 -2.3504320E-01 1.9231613E-01 4.4583201E-02 -3.3447982E-02 -4.0980859E-02 -2.4840415E-02 -1.2463954E-02 -2.4840415E-02 -1.2463954E-03 -2.6582428E-03 -2.6582428E-03 -1.2847058E-03 -3.4899562E-04 -1.8822394E-04 -1.8622394E-04 -1.8025504E-05 -3.3429305E-06 -9.4676609E-08 -1.4244408E-07 2.184245E-06 -1.4244408E-07 -1.4244408E-06 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.4244408E-07 -1.424408E	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 1.3477866E-01 -6.6197533E-02 3.6084562E-02 5.1750801E-02 1.1943673E-02 -8.806305E-03 -1.0840501E-02 -1.943673E-03 -3.2936776E-03 -1.5028703E-03 -1.5028703E-04 -3.3918314E-04 -1.7412861E-04 -3.3918314E-04 -1.7412861E-04 -3.3918314E-04 -1.7412861E-04 -2.49699458E-05 -2.6471634E-05 -1.3792011E-05 -6.7358838E-06 -3.0106423E-06 -8.8262848E-07 -2.4999155E-08	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 173\\ 174\\ 175\\ 176\\ 176\\ 177\\ 178\\ 181\\ 182\\ 183\\ 184\\ 185\\ 183\\ 184\\ 185\\ 188\\ 185\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ 198\\ 199\\ 200\\ 201\\ 202\\ 202$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3733139E-00 2.5427420E+00 1.6203217E+01 3.0302910E+01 5.7066236E+01 1.0845021E+02 2.0847323E+02 4.0651542E+02 8.0667635E+02 1.6308164E+04 3.3966005E+03 7.2674336E+03 1.6690414E+06 4.8762050E+04 8.8762050E+04 1.6592545E+07 5.4660323E+07 2.0153596E+08 3.5433483E-02 6.5194589E-02 1.995578E-01 1.995578E-01 1.995578E-01	-2.1110836E-06 8.2038732E-06 3.2465036E-05 -5.0544404E-05 7.5145363E-04 -1.939967E-04 1.8953650E-04 -3.7221586E-04 9.7479204E-04 2.2886884E-02 1.5476535E-01 3.1357302E-01 2.0254912E-01 1.0544176E-01 5.0059648E-02 2.3694166E-02 2.3694166E-02 1.638547E-02 1.638547E-02 1.638547E-02 1.038547E-04 2.31931225E-03 3.1931225E-03 3.1931225E-04 3.1931225E-04 3.0692464E-05 8.6822796E-07 -8.5886264E-06 4.8437004E-06 -1.4154628E-05	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 1.1223456E-03 1.5950138E-03 -2.0117491E-03 2.2268120E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -4.2069238E-01 -4.2069238E-01 1.6311570E-01 1.6311570E-01 1.8279811E-01 1.1347400E-01 1.8279811E-01 1.3241258E-02 2.6435568E-02 1.2341258E-02 2.6435568E-02 1.2341258E-03 3.0784422E-03 1.6331902E-03 8.8035369E-04 4.6333992E-04 2.3446020E-04 1.1943149E-04 5.3372488E-05 1.5649976E-05 4.4288491E-07 -3.8710980E-08 -2.3081520E-07 6.9349778E-07 9.9092778E-07	8.2318337E-05 -3.222822E-04 7.070295E-01 -1.2533334E-03 1.8997745E-03 2.6453479E-03 5.1813384E-03 2.1606845E-02 2.6654648E-01 3.4575529E-01 -3.0935771E-01 -4.003806E-01 9.4601050E-02 2.9134598E-02 1.3361681E-02 6.2310645E-03 3.0182407E-03 1.5480068E-03 8.1995336E-04 1.2269895E-04 1.2269895E-04 1.2269895E-04 1.2269895E-05 7.8534060E-06 2.2234096E-07 -1.3229008E-06 1.4609437E-07 -3.8764579E-07 -3.8764579E-07	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 4.8490218E-01 -1.0409201E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 4.4583201E-02 -3.3447982E-02 -2.4840415E-02 -1.2463954E-02 -2.4840415E-02 -1.2463954E-03 -2.6582428E-03 -1.2847058E-04 -3.4899562E-04 -3.4899562E-04 -1.802544E-05 -3.3429305E-06 -9.4676609E-08 -1.4244408E-07 -1.1864265E-06 -4.0988158E-06 -4.0988158E-06 -1.402854E-04 -1.864255E-06 -1.402854E-06 -1.4028555555555555555555555555555555555555	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 3.6084562E-02 3.6084562E-02 1.1943673E-02 -5.1750801E-02 -6.5613532E-03 -7.0213261E-04 -3.3918314E-04 -1.7415861E-04 -9.2142104E-05 -4.9699458E-03 -1.741581E-04 -9.2142104E-05 -6.7358838E-07 -3.3016423E-08 -8.8262848E-07 -2.4999155E-08 -1.4597307E-04 -5.1850903E-04 -1.4597307E-04 -5.1850903E-04 -1.0854283E-03	
$\begin{array}{c} 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 177\\ 178\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 188\\ 186\\ 187\\ 188\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 193\\ 194\\ 195\\ 196\\ 197\\ 199\\ 200\\ 201\\ 202\\ 203\\ 204\\ \end{array}$	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3733189E-00 2.5427420E+00 8.7095624E+00 1.6203217E+01 3.0302910E+01 5.7068236E+01 1.0845021E+02 2.0847332E+02 1.6348107E+03 3.3969006E+03 7.2674336E+03 1.6080864E+04 8.8762050E+04 2.335591E+05 5.9356338E+05 1.6690414E+06 4.9925105E+06 1.552556E+07 2.0153596E+08 3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01	-2.1110836E-06 8.2038732E-06 1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-04 1.9393650E-04 -1.9393967E-04 1.8953650E-04 9.7479204E-04 9.7479204E-04 2.2896984E-02 1.5476535E-01 3.1357302E-01 2.0254912E-01 1.0544176E-01 2.054912E-01 1.0544176E-02 1.638547E-02 2.3694166E-02 1.638547E-02 3.1931225E-03 1.7276138E-03 9.1977675E-04 3.0692464E-05 8.6822796E-07 -8.5886264E-06 4.8437004E-06 -1.4154628E-05 -2.5120815E-06	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 1.5950138E-03 -2.0117491E-03 2.208120E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -4.9060947E-01 -1.0565728E-01 1.6311570E-01 1.63279811E-01 1.1347400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 6.0023349E-03 3.0764422E-03 1.6331902E-03 8.8035369E-04 4.6933992E-04 2.4446020E-04 1.549976E-05 4.4288491E-07 -3.8710980E-08 -2.3081520E-07 6.9349778E-07 -2.0262797E-06	8.2318337E-05 -3.2228822E-04 7.070285E-03 1.253334E-03 1.8997745E-03 -2.6453479E-03 2.1606845E-02 2.6654648E-01 3.4575529E-01 -3.0935771E-01 -9.4601050E-02 7.9749840E-02 2.9134598E-02 5.8154906E-02 2.9134598E-02 5.8154906E-02 2.9134598E-02 5.8154906E-03 3.0182407E-03 3.0182407E-03 3.0182407E-03 3.158502E-04 4.202932E-04 5.269985E-04 5.269895E-04 5.2678502E-05 7.8534060E-06 2.2234096E-07 -1.3229008E-06 1.4609437E-07 -3.8764579E-07 -3.8764579E-07 -5.2597042E-04	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 -3.0964189E-01 4.8490218E-01 -1.0409201E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 4.4583201E-02 -3.3447982E-02 -2.4840415E-02 -1.2463954E-02 -2.4840415E-02 -1.2463954E-03 -2.6582428E-03 -2.6582428E-03 -1.2847058E-03 -3.4899562E-04 -1.0026146E-04 -5.235504E-05 -3.3429305E-06 -9.4676609E-08 -1.4244408E-07 -2.1864265E-06 -4.0988158E-06 -4.0988158E-06 -2.488258E-05 -3.289562E-04 -3.488258E-05 -3.488258E-05 -4.0988158E-06 -4.0988158E-06 -2.888258E-05 -3.488258E-05 -3.488258E-05 -4.0988158E-06 -4.0988258E-05 -4.0988258E-0	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 .0051539E-01 1.8040757E-01 -2.2131882E-02 3.6084562E-02 3.6084562E-02 5.1750801E-02 1.1943673E-03 -8.8056305E-03 -1.0845051E-02 -6.5613532E-03 -1.0845051E-04 -3.3918314E-04 -9.2142104E-05 -1.3792011E-05 -6.7358382E-06 -3.0106423E-08 -8.8262848E-07 -2.4999155E-08 -1.4597307E-04 -5.1850903E-04 -1.0824528-03 -1.0824528-03 -1.0824528-03 -1.0824528-03 -1.0824528-03 -1.0824528-03 -1.0824528-03 -1.0824528E-03 -1.08549307E-04 -1.0854283E-03 -1.0824282E-03 -1.08248282E-03	
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168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 200 201 202 203 204 205 206 207 208 209 210 211 212 212	3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01 4.0626020E-01 1.3783189E+00 2.5427420E+00 1.6203217E+01 3.0302910E+01 1.0845021E+02 2.0847332E+02 2.0847332E+02 2.0847332E+02 2.0847332E+02 3.03667635E+02 1.6348107E+03 3.3369005E+03 7.2674336E+03 1.660864E+04 4.3674132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05 1.6690414E+06 4.9925105E+06 1.5952595E+07 5.4660323E+07 2.0153596E+08 3.5433483E-02 6.5194589E-01 2.2073350E-01 4.0626020E+01 1.3783189E+00 2.5427420E+00 4.5995778E+00 8.7095624E+00 1.6203217E+01 3.302910E+01 5.7066236E+01	-2.1110836E-06 8.2038732E-06 -1.8429299E-05 3.2465036E-05 -5.0544404E-05 7.5145363E-05 -1.0224235E-04 -1.9339967E-04 1.8953650E-04 9.7479204E-04 2.2896984E-02 1.5476535E-01 3.1765576E-01 3.1357302E-01 2.0254912E-01 1.0544176E-01 2.0254912E-01 1.0544176E-02 2.369416E-02 2.369416E-02 2.369416E-02 2.369416E-02 3.1931225E-03 3.1931225E-03 3.1931225E-03 3.192765E-04 4.7923133E-04 2.3419075E-04 3.0692464E-05 8.6822796E-07 -8.5886264E-06 4.8437004E-06 2.5120815E-06 -2.001927E-05 -4.0436086E-05 -5.4843802E-05 -5.4843802E-05 -5.4843802E-05 -1.4154628E-05 -9.7950298E-05 -1.4327167E-04 -3.4077759E-04 8.0186654E-04	3.3329049E-05 -1.2966616E-04 2.8944290E-04 -5.0746384E-04 7.8669527E-04 -1.1223456E-03 -2.0117491E-03 2.208120E-03 9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -9.3713975E-03 -1.0565728E-01 1.6311570E-01 1.63279811E-01 1.1347400E-01 5.7122173E-02 2.6435568E-02 1.2341259E-02 2.6435568E-02 1.2341259E-02 2.6435568E-02 1.2341259E-02 3.0784422E-03 1.6331902E-03 3.03748422E-03 1.6331902E-04 2.3446020E-04 1.1943149E-04 4.693392E-04 2.4446020E-04 1.549976E-05 4.4288491E-07 -3.8710980E-08 -2.0262797E-06 3.9614954E-06 1.5053840E-05 -2.7098584E-05 -2.2084376E-04 -3.2178309E-03 .8804793E-05 -2.2834376E-04 -3.2178309E-03 .1.9221810E-02 -3.0239516E-02	8.2318337E-05 -3.222822E-04 7.070285E-03 1.2533334E-03 1.8997745E-03 2.6453479E-03 2.1606845E-02 2.6654648E-01 3.4575529E-01 -3.0935771E-01 -4.0033696E-01 -9.4601050E-02 9.520998E-02 5.8154906E-02 2.9134598E-02 2.9134598E-02 2.9134598E-02 2.9134598E-02 3.0182407E-03 3.15480068E-03 3.1985336E-04 4.4204912E-04 4.2269895E-04 5.9934273E-05 2.6785502E-05 2.6785502E-05 2.776505E-04 4.2962105E-05 2.7176505E-04 4.703211E-03 1.4966814E-02 1.306508E-02 2.1306558E-04 1.3306508E-02 2.1306558E-04 1.3306558E-02 2.24603559E-04 1.3306558E-02 2.24603559E-04 1.3306558E-02 2.24603559E-04 1.3306558E-02 2.24603559E-04 1.3306559E-04 1.3306559	-2.3099532E-04 1.1078969E-03 -1.5754355E-03 2.6096020E-02 2.1315146E-01 5.0964189E-01 4.8490218E-01 -2.3504320E-01 1.3640741E-01 1.9231613E-01 4.4583201E-02 -3.3447982E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-02 -2.4840415E-02 -2.65913307E-03 -2.6582428E-03 -1.2847058E-03 -3.4899562E-04 -1.822394E-04 -1.822394E-04 -1.822394E-04 -1.822394E-04 -1.4244408E-07 2.158426E-05 -3.3429305E-06 -3.4899562E-04 -1.4244408E-07 2.1864265E-06 -3.489258E-06 -3.4299562E-03 -1.4244408E-07 2.1864265E-06 -3.429305E-06 -3.429305E-06 -3.429305E-06 -1.42944208E-07 2.1864265E-06 -3.3429305E-06 -3.488258E-05 1.5246689E-03 4.8629178E-03 6.396013E-03 -1.183559E-02 -7.6887039E-03 6.1499391E-03 1.1813559E-02	-9.5114313E-02 -2.4887441E-01 -3.8418187E-01 -3.1103172E-01 -1.4702572E-01 7.3403494E-02 2.0051539E-01 1.8040757E-01 -2.2131882E-02 3.6084562E-02 5.1750801E-02 1.943673E-02 -8.8056305E-03 -1.0840501E-02 -6.5613532E-03 -1.0840501E-02 -6.5613532E-03 -1.282703E-03 -1.5028703E-03 -7.0213261E-04 -3.3918314E-04 -9.2142104E-05 -4.9699458E-05 -2.6471634E-04 -9.2142104E-05 -4.9699458E-05 -2.6471634E-04 -9.2142104E-05 -4.9699458E-05 -2.6471634E-04 -3.0106423E-06 -3.0106423E-06 -3.0106423E-08 -1.0854238E-03 -1.1921947E-03 -1.085428E-03 -1.1921947E-03 -3.9119711E-04 -3.2417362E-04 1.9209398E-03 2.3470890E-03 2.3470890E-03 2.3470890E-03 2.3470890E-03 2.3470890E-03 2.34718740E-04 -3.178740E-04 -3.178740E-03	

214	2.0847323E+02	3.5937378E-02	1.8702867E-02	9.1824211E-03	-3.8549441E-03 -1.0150111E-03
215	4.0651542E+02	4.8738390E-02	2.8588551E-02	1.4912210E-02	-6.4213853E-03 -1.6987496E-03
216	8.0667635E+02	4.2344757E-02	2.3814232E-02	1.2212514E-02	-5.2165181E-03 -1.3778789E-03
217	1.6348107E+03	2.8772905E-02	1.5644329E-02	7.9877030E-03	-3,4187444E-03 -9,0350250E-04
218	3 3969005F+03	1 6986116E-02	9 0076332F-03	4 5551383E-03	-1 9399597F-03 -5 1219513F-04
210	7 06742268+02	0 26502055-02	4 0076020E-02	0 4000607E_02	-1 0602E12E-02 -2 9010111E-04
219	1.2074330E+03	9.3036323E-03	4.9070239E-03	2.4020007E-03	-1.0002513E-03 -2.8010111E-04
220	1.60808645+04	4.9669445E-03	2.5660416E-03	1.3021501E-03	-5.5395659E-04 -1.4623361E-04
221	3.6974132E+04	2.6253728E-03	1.3570783E-03	6.8425087E-04	-2.9193075E-04 -7.7112040E-05
222	8.8762050E+04	1.3744607E-03	7.0676310E-04	3.5489843E-04	-1.5093380E-04 -3.9842201E-05
223	2.2355921E+05	7.1797657E-04	3.6856498E-04	1.8548117E-04	-7.9083365E-05 -2.0887093E-05
224	5.9356339E+05	3.7046632E-04	1.8956211E-04	9.5105240E-05	-4.0448225E-05 -1.0677407E-05
225	1.6690414E+06	1.8661865E-04	9.5434683E-05	4.7970253E-05	-2.0442610E-05 -5.3986815E-06
226	4.9925105E+06	8.8855319E-05	4.5355929E-05	2.2748343E-05	-9.6761026E-06 -2.5543594E-06
227	1.5952595E+07	3.7642546E-05	1.9216236E-05	9.6534660E-06	-4.1127730E-06 -1.0860871E-06
228	5.4660323E+07	1.0702166E-05	5.4565863E-06	2.7355003E-06	-1.1632623E-06 -3.0707008E-07
229	2.0153596E+08	3.3837491E-07	1.7331530E-07	8.7896073E-08	-3.7781680E-08 -9.9958460E-09
230					
231					
201		20+	20+	4D+	ED+ CD+
202		-4 9090010E+00	-1 14E02EEE+00	-0 4606400E+01	-2 E026007E+00 -0 108800EE-01
200		4.02033131102	1.14000001.02	2.40304301101	5.55502271100 2.15000231 01
234					
230					
236	3.5433483E-02	-1.6353670E-06	3.0868694E-05	-1.1864655E-04	1.5855754E-04 -2.1084460E-01
237	6.5194589E-02	6.3316603E-06	-1.2026428E-04	4.6694629E-04	-1.2548766E-03 -2.8111761E-01
238	1.1995578E-01	-1.4219884E-05	2.6796577E-04	-1.0180223E-03	1.0820358E-03 -3.9737451E-01
239	2.2073350E-01	2.4992100E-05	-4.6903534E-04	1.7890741E-03	-1.0206289E-02 -2.2012706E-01
240	4.0626020E-01	-3.8612896E-05	7.2606778E-04	-2.6931726E-03	-5.9228112E-02 -7.0584944E-02
241	7.4802875E-01	5.7574583E-05	-1.0210499E-03	3.4705786E-03	-3.0443611E-01 1.2807543E-01
242	1.3783189E+00	-7.5089141E-05	1.4700244E-03	-8.3211961E-03	-5.4484929E-01 1.8731223E-01
243	2.5427420E+00	1.0885749E-04	-1.7738974E-03	-5.0169252E-02	-3.5977524E-01 1.2136805E-01
244	4 6995778F+00	-1 3997879F-04	1 6176208E-03	-3 7440022E-01	2 5348989F-01 -6 5756816F-02
245	8 7095624E+00	6 156/771E-05	-1 7286003E-02	-6 3300409E-01	A 4847514E-01 -1 1845734E-01
240	1 6003017E+01	1 0053100E 04	1.7200003E 02	1 7504401E 01	1.0440142E 01 2.0527052E 02
240	1.62032178+01	-1.9253162E-04	-1.6403996E-01	-1.7564461E-01	1.2440143E-01 -3.2537953E-02
247	3.0302910E+01	1.9618065E-03	-5.0777453E-01	4.1846218E-01	-1.9083216E-01 4.7187098E-02
248	5.7068236E+01	4.7503498E-02	-4.2382810E-01	3.4505648E-01	-1.6162607E-01 4.0084398E-02
249	1.0845021E+02	2.2099001E-01	1.4577962E-02	1.4811851E-02	-8.1127462E-03 2.0606073E-03
250	2.0847323E+02	3.5443326E-01	2.1417794E-01	-1.1076659E-01	4.6283226E-02 -1.1300549E-02
251	4.0651542E+02	2.8912370E-01	1.7573134E-01	-9.2133021E-02	3.8900389E-02 -9.5072685E-03
252	8.0667635E+02	1.5637333E-01	9.0065826E-02	-4.6295924E-02	1.9377585E-02 -4.7315319E-03
253	1.6348107E+03	6.6617703E-02	3.7175835E-02	-1.9041634E-02	7.9919236E-03 -1.9516142E-03
254	3.3969005E+03	2.4461997E-02	1.3316345E-02	-6.7495936E-03	2.8159453E-03 -6.8726177E-04
255	7.2674336E+03	8.2393379E-03	4.4493450E-03	-2.2612571E-03	9.4762317E-04 -2.3135097E-04
256	1.6080864E+04	2.6125442E-03	1.3961041E-03	-7.0410062E-04	2.9329310E-04 -7.1567591E-05
257	3 6974132E+04	7 9905759E-04	4 2714895E-04	-2 1667865E-04	9 0808371E-05 -2 2169026E-05
258	8.8762050E+04	2.3721957E-04	1.2581238E-04	-6.3293550E-05	2 6335175E-05 -6 4253996E-06
250	2 2355921E+05	6 91/17/3E-05	3 6785036E-05	-1 8651687E-05	7 8206540E-06 -1 9092936E-06
260	5 9356339F+05	1 9622230F-05	1 0354569E-05	-5 1982446E-06	2 1602316E-06 -5 2700445E-07
200	1 6600414E+06	E 4040046E-06	0.0701060E_06	-1 4600197E-06	6 100EE99E-07 -1 406EE40E-07
201	1.0090414E+00	5.4240040E-00	2.0701002E-00	-1.4002107E-00	0.1295568E-07 -1.4905542E-07
202	4.99251056+06	1.4307210E-06	1.510/101E-0/	-3.7635023E-07	1.5003/52E-0/ -3.8056963E-08
203	1.5952595E+07	3.5694444E-07	1.8952330E-07	-9.6468/44E-08	4.0629470E-08 -9.9224055E-09
264	5.4660323E+07	7.8336742E-08	4.0935008E-08	-2.0342964E-08	8.3784907E-09 -2.0424753E-09
265	2.0153596E+08	4.7974022E-09	2.6197636E-09	-1.3906157E-09	6.0777694E-10 -1.4885981E-10
266					
267					
268	3.5433483E-02	-3.3155956E-09	5.3478695E-08	-1.8607538E-07	2.4510510E-07 -3.2381110E-04
269	6.5194589E-02	1.6117769E-08	-2.7246598E-07	9.8672929E-07	-2.6198936E-06 -5.8561740E-04
270	1.1995578E-01	-4.6595294E-08	8.0476637E-07	-2.9071371E-06	3.0698562E-06 -1.1228754E-03
271	2.2073350E-01	1.0721820E-07	-1.8815173E-06	6.9116575E-06	-3.9145196E-05 -8.4376525E-04
272	4.0626020E-01	-2.1931450E-07	3.9092356E-06	-1.4091566E-05	-3.0799063E-04 -3.6704690E-04
273	7.4802875E-01	4.3505976E-07	-7.4083076E-06	2.4621994E-05	-2.1484003E-03 9.0376973E-04
274	1.3783189E+00	-7.6294621E-07	1.4383728E-05	-7.9917296E-05	-5.2189035E-03 1.7940892E-03
275	2.5427420E+00	1.4824094E-06	-2.3519099E-05	-6.5281515E-04	-4.6799819E-03 1.5786549E-03
276	4.6995778E+00	-2.5722484E-06	2.9232619E-05	-6.6255565E-03	4.4850584E-03 -1.1635075E-03
277	8.7095624E+00	1.6116575E-06	-4.1795075E-04	-1.5241335E-02	1.0793797E-02 -2.8508509E-03
278	1.6203217E+01	-6.4987104E-06	-5.3992894E-03	-5.7571411E-03	4.0723665E-03 -1.0651199E-03
279	3.0302910E+01	8.9154726E-05	-2.2837477E-02	1.8797085E-02	-8.5717355E-03 2.1195362E-03
280	5.7068236E+01	2.9590464E-03	-2.6050224E-02	2.1169534E-02	-9.9123723E-03 2.4582134E-03
281	1 0845021F+02	1 8924339E-02	1 3746655E-03	1 1499728F-03	-6 3925869F-04 1 6268677F-04
282	2 0847323F+02	4 1819595E-02	2 5124039E-02	-1 2984778E-02	5 4250241F-03 -1 3245584F-03
283	A 0651542E+02	4.1010000E 02	2.0124000E 02	-1 /8//976E-02	6 2656237E-03 -1 5312301E-03
200	9.066762EE+02	2 E114720E-00	2.0004030E 02	-1 0072060E-00	4 207E2EEE_02 -1 0402687E_02
204	1.62401035E+02	3.5114/32E-02	1 12700525 00	-1.02/3208E-02	4.2975255E-03 -1.0492087E-03
200	1.63461076+03	2.0591420E-02	1.1372953E-02	-5.0119902E-03	2.4363402E-03 -5.9539763E-04
280	3.3969005E+03	1.0336508E-02	5.5656545E-03	-2.8130957E-03	1.1726399E-03 -2.8616504E-04
287	7.2674336E+03	4.7071277E-03	2.5160046E-03	-1.2761248E-03	5.3473105E-04 -1.3054238E-04
288	1.6080864E+04	1.9803439E-03	1.04/1764E-03	-5.2638914E-04	2.1895806E-04 -5.3420806E-05
289	3.6974132E+04	1.8378096E-04	4.1574989E-04	-2.1078545E-04	8.8425502E-05 -2.1588333E-05
290	8.8762050E+04	2.9062695E-04	1.5274519E-04	-7.6497777E-05	3.1733883E-05 -7.7405204E-06
291	2.2355921E+05	1.0196314E-04	5.4097845E-05	-2.7514113E-05	1.1580086E-05 -2.8278961E-06
292	5.9356339E+05	3.3260336E-05	1.7397118E-05	-8.6605403E-06	3.5729027E-06 -8.7110633E-07
293	1.6690414E+06	1.0232548E-05	5.4559496E-06	-2.7975585E-06	1.1862834E-06 -2.8986653E-07
294	4.9925105E+06	2.8704711E-06	1.4875248E-06	-7.2996545E-07	2.9700737E-07 -7.2330628E-08
295	1.5952595E+07	7.5427076E-07	4.0779464E-07	-2.1343459E-07	9.2166263E-08 -2.2552841E-08
296	5.4660323E+07	1.4613123E-07	7.3243809E-08	-3.3993336E-08	1.3052326E-08 -3.1629306E-09
297	2.0153596E+08	1.9315900E-09	2.1567584E-09	-1.9670922E-09	1.1635497E-09 -2.9069129E-10
298					
200					
300		3D-	<u>4</u> ۵–	50-	
301		-9 68106405+01	-1 69195505-01	-1 13860/05+00	
303		3.0010042E+01	1.03100005401	1.12002405+00	
302					
204	2 E400400E CC	7 57040000 00	4 20620200 05	7 00000000 05	
304	3.5433483E-02	1.5/84238E-06	4.320/2/0E-05	1.8236958E-05	
305	0.5194589E-02	-∠.0993559E-05	-1.5341514E-04	-1.000/136E-03	

306	1.1995578E-01	5.7267393E-05	3.1485487E-04	-7.3354507E-03
307	2.2073350E-01	-9.8181660E-05	-5.4111707E-04	-5.5260441E-02
308	4.0626020E-01	1.5037695E-04	7.8310505E-04	-1.7246183E-01
309	7.4802875E-01	-2.1738056E-04	-8.3176454E-04	-3.2770786E-01
310	1.3783189E+00	3.0219815E-04	6.3470740E-03	-3.8344465E-01
311	2.5427420E+00	-4.4994548E-04	5.7171355E-02	-2.4878259E-01
312	4.6995778E+00	3.9049198E-05	2.6346697E-01	4.0375292E-02
313	8.7095624E+00	-8.0122761E-03	4.5805697E-01	2.0149629E-01
314	1.6203217E+01	-7.4226625E-02	3.3001447E-01	1.4691305E-01
310	3.0302910E+01	-2.5949707E-01	-6.3462926E-03	1.1012835E-02
317	1 0845021E+02	-3.7200015E-01	-1.0090131E-01	-6.5016978E-02
318	2 0847323E+02	-2.01/1109E-01	-7.8386764E-02	-2 7/69/77E-02
310	4 0651542F+02	-5 4081638F-02	-2 9251770F-02	-1 0187547E-02
320	8.0667635E+02	-1.7643813E-02	-9.4798446E-03	-3.3057717E-03
321	1.6348107E+03	-5.2335178E-03	-2.7774063E-03	-9.6304002E-04
322	3.3969005E+03	-1.5325460E-03	-8.1584319E-04	-2.8426295E-04
323	7.2674336E+03	-4.6095060E-04	-2.4259466E-04	-8.3902621E-05
324	1.6080864E+04	-1.4789734E-04	-7.8497956E-05	-2.7352488E-05
325	3.6974132E+04	-4.7671984E-05	-2.5017391E-05	-8.6454048E-06
326	8.8762050E+04	-1.6984983E-05	-8.9980573E-06	-3.1333861E-06
327	2.2355921E+05	-4.5486942E-06	-2.3853540E-06	-8.2421615E-07
328	5.9356339E+05	-2.4306190E-06	-1.2844651E-06	-4.4653051E-07
329				
330	2 54224025 00	6 6070004E 00		1 50447055 07
331	3.3433483E-02 6 5194589E-02	-5 5134212E-00	-3 8586569E-07	-2 6097866E-04
334 332	1 19955785-01	3 32081/55-07	9 7973560E-07	-2 4484243E-05
334	2.2073350F-01	-2.5675922F-07	-2.5626833F-06	-2.5057139F-04
335	4.0626020E-01	1.4400230E-06	4.5493849E-06	-1.0610208E-03
336	7.4802875E-01	-8.2919598E-07	-7.4959695E-06	-2.7357957E-03
337	1.3783189E+00	5.6902067E-06	7.0748212E-05	-4.3450043E-03
338	2.5427420E+00	-2.2419726E-06	8.7781103E-04	-3.8281416E-03
339	4.6995778E+00	1.1210953E-05	5.5097183E-03	8.4595301E-04
340	8.7095624E+00	-2.0650628E-04	1.3039108E-02	5.7362336E-03
341	1.6203217E+01	-2.8411004E-03	1.2798368E-02	5.6966163E-03
342	3.0302910E+01	-1.3701878E-02	-3.4945280E-04	5.7576690E-04
343	5.7068236E+01	-2.6948928E-02	-1.3689346E-02	-4.7117273E-03
344	1.0845021E+02	-2.7850497E-02	-1.5316871E-02	-5.3508675E-03
345	2.0847323E+02	-1.9120857E-02	-1.0566583E-02	-3.7033238E-03
346	4.0651542E+02	-9.8424297E-03	-5.3236691E-03	-1.8539306E-03
347	8.066/635E+02	-4.24/6636E-03	-2.2836292E-03	-7.9658186E-04
348	1.6348107E+03	-1.6035530E-03	-8.5066614E-04	-2.94/925/E-04
349	3.3969005E+03	-5.020/220E-04	-3.0040066E-04	-1.0404029E-04 -3.3782723E-05
000	1.20143306103	1.00001035 04	3.00130201 03	0.01021206 00
351	1 6080864F+04	-6 0891217F-05	-3 2665057F-05	-1 1464903E-05
351 352	1.6080864E+04 3.6974132E+04	-6.0891217E-05	-3.2665057E-05	-1.1464903E-05
351 352 353	1.6080864E+04 3.6974132E+04 8.8762050E+04	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06
351 352 353 354	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07
351 352 353 354 355	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06 -6.4693359E-07	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07
351 352 353 354 355 356	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06 -6.4693359E-07	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07
351 352 353 354 355 356 357	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06 -6.4693359E-07	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07
351 352 353 354 355 356 356 357 358	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06 -6.4693359E-07 3D+	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07 4D+	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07
351 352 353 354 355 356 357 358 359 260	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06 -6.4693359E-07 3D+ -9.2970175E+01	-3.2265057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07 4D+ -1.6065511E+01	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07 -1.0359352E+00
351 352 353 354 355 356 357 358 359 360 261	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05	-6.0891217E-05 -1.8933714E-05 -6.0219306E-06 -1.6877326E-06 -6.4693359E-07 -9.2970175E+01	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07 -4D+ -1.6065511E+01	-1.1464903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07 -1.0359352E+00
351 352 353 354 355 356 357 358 359 360 361 362	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05	-6.0891217E-05 -0.219396E-06 -0.219396E-06 -1.6877326E-06 -6.4693359E-07 3D+ -9.2970175E+01 7.7221792E-06	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07 -4D+ -1.6065511E+01 -4.6214141E-05	-1.164903E-05 -3.3354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07 -1.0359352E+00 2.1952461E-05
351 352 353 354 355 356 357 358 359 360 361 362 363	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05 3.5433483E-02 6.5194588E-02	-6.0891217E-05 -0.219396E-06 -0.219396E-06 -1.6877326E-06 -6.4693359E-07 3D+ -9.2970175E+01 7.7221792E-06 -2.7509786E-05	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07 4D+ -1.6065511E+01 4.6214141E-05 -1.6424473E-04	-1.1464903E-05 -3.3354802E-06 -1.165944E-06 -2.8284055E-07 -1.2693531E-07 -1.0359352E+00 2.1952461E-05 -1.4251127E-03
351 352 353 354 355 356 357 358 359 360 361 362 363 364	1.6080864E+04 3.6974132E+04 8.8762050E+04 2.2355921E+05 5.9356339E+05 3.5433483E-02 6.5194589E-02 1.199578E-01	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06 -6.4693359E-07 -9.2970175E+01 7.7221792E-06 -2.7509786E-05 5.8345961E-05	-3.2665057E-05 -9.7813981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07 4D+ -1.6065511E+01 4.6214141E-05 -1.6424473E-04 3.3612523E-04	-1.164903E-05 -3.3354802E-06 -1.165944E-06 -2.8284055E-07 -1.2693531E-07 -1.0359352E+00 2.1952461E-05 -1.4251127E-03 -1.0625745E-02
351 352 353 354 355 356 357 358 359 360 361 362 363 364 365	1.6080864E+04 3.6974132E+04 2.2355921E+05 5.9356339E+05 3.5433483E-02 6.5194589E-02 1.1995578E-01 2.2073350E-01	-6.0891217E-05 -1.8933714E-05 -6.0219396E-06 -1.6877326E-06 -6.4693359E-07 3D+ -9.2970175E+01 7.7221792E-06 -2.7509786E-05 5.8345961E-05 5.8345961E-05 9.9974735E-05	-3.2665057E-05 -9.7613981E-06 -3.2810341E-06 -8.4801421E-07 -3.5510080E-07 -1.6065511E+01 -1.6065511E+01 -1.6424473E-04 3.3612523E-04 -5.7481198E-04	-1.164903E-05 -3.354802E-06 -1.1659544E-06 -2.8284055E-07 -1.2693531E-07 -1.2693531E-07 -1.0359352E+00 2.1952461E-05 -1.4251127E-03 -1.0625745E-02 -6.7684218E-02
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427	2.5427420E+00 -1.0821454E-0	1
428	4.6995778E+00 -2.3593616E-0	1
429	8.7095624E+00 -3.2184810E-0	1
430	1.6203217E+01 -2.9865700E-0	1
431	3.0302910E+01 -1.9561991E-0	1
432	5.7068236E+01 -8.8370628E-0	2
433	1.0845021E+02 -3.0872542E-0	2
434	2.0847323E+02 -8.4857068E-0	3
435	4.0651542E+02 -1.9423015E-0	3
436	8.0667635E+02 -4.1900690E-0	4
437	1.6348107E+03 -8.3141076E-0	5
438	3.3969005E+03 -1.5517453E-0	5
439	7.2674336E+03 -4.6868130E-0	6
440		-
441		
442	3.5433483E-02 -3.0184033E-0	8
443	6.5194589E-02 1.4123331E-0	7
444	1.1995578E-01 -3.6812892E-0	7
445	2.2073350E-01 6.5493014E-0	7
446	4 0626020E-01 -3 9507151E-0	6
447	7.4802875E-01 -3.4920504E-0	5
448	1.3783189E+00 -3.8022076E-0	4
449	2.5427420E+00 -1.8871046E-0	3
450	4.6995778E+00 -5.5934358E-0	3
451	8.7095624E+00 -1.0381556E-0	2
452	1.6203217E+01 -1.3122465E-0	2
453	3.0302910E+01 -1.1720703E-0	2
454	5.7068236E+01 -7.2258794E-0	3
455	1.0845021E+02 -3.4399092E-0	3
456	2.0847323E+02 -1.2821405E-0	3
457	4.0651542E+02 -3.9287197E-0	4
458	8.0667635E+02 -1.1098769E-0	4
459	1.6348107E+03 -2.6812267E-0	5
460	3.3969005E+03 -6.3265217E-0	6
461	7.2674336E+03 -1.6293580E-0	6
462		
463		
464	4F	+
465	-5.7413469E+0	0
466		
467		
468	3.5433483E-02 -1.5556098E-0	5
469	6.5194589E-02 4.9990333E-0	5
470	1.1995578E-01 -1.0088117E-0	4
471	2.2073350E-01 1.1518582E-0	4
472	4.0626020E-01 -6.4369648E-0	4
473	7.4802875E-01 -4.2360900E-0	3
474	1.3783189E+00 -3.1861324E-0	2
475	2.5427420E+00 -1.1273317E-0	1
476	4.6995778E+00 -2.4091820E-0	1
477	8.7095624E+00 -3.2341441E-0	1
478	1.6203217E+01 -2.9517418E-0	1
479	3.0302910E+01 -1.9089221E-0	1
480	5.7068236E+01 -8.5166804E-0	2
481	1.0845021E+02 -2.9037579E-0	2
482	2.0847323E+02 -7.7172949E-0	3
483	4.0651542E+02 -1.6767727E-0	3
484	8.0667635E+02 -3.3097325E-0	4
485	1.6348107E+03 -5.4957097E-0	5
486	3.3969005E+03 -8.8754940E-0	6
487	7.2674336E+03 -1.4989268E-0	6
488		
489		

490	3.5433483E-02 -3.2617168E-08
491	6.5194589E-02 1.4149420E-07
492	1.1995578E-01 -3.8604183E-07
493	4.0626020E-01 -4.5010270E-06
495	7.4802875E-01 -4.0093122E-05
496	1.3783189E+00 -4.0951459E-04
497	2.5427420E+00 -1.9678245E-03
498	4.0995776E+00 -5.7167356E-03 8.7095624E+00 -1.0444036E-02
500	1.6203217E+01 -1.2993386E-02
501	3.0302910E+01 -1.1476039E-02
502	5.7068236E+01 -7.0050481E-03
504	2.0847323E+02 -1.1959300E-03
505	4.0651542E+02 -3.5705524E-04
506	8.0667635E+02 -9.7043968E-05
508	1.6348107E+03 -2.1994873E-05 3.3969005E+03 -4.9229745E-06
509	7.2674336E+03 -1.0697561E-06
510	
511	
513	Literature energy = $-2.0913713216718592E+04$
514	Difference (cal - lit) = 1.12E-03
515	Relative error (abs((cal - lit)/lit)) = 5.33E-08
516 517	Basis set for original program
518	3.543348300000002E-02 1.0d0 1.0d0
519	6.5194588593144476E-02 1.0d0 1.0d0
520	1.1995577607433897E-01 1.0d0 1.0d0
521 522	2.2073349755341545E-01 1.0d0 1.0d0 4.0626019965028504E-01 1.0d0 1.0d0
523	7.4802874797813979E-01 1.0d0 1.0d0
524	1.3783189024559244E+00 1.0d0 1.0d0
525	2.5427420408376111E+00 1.0d0 1.0d0
527	4.6995776531749465E+00 1.0d0 1.0d0 8.7095624280738555E+00 1.0d0 1.0d0
528	1.6203216735620309E+01 1.0d0 1.0d0
529	3.0302909733749487E+01 1.0d0 1.0d0
530	5.7068235542655763E+01 1.0d0 1.0d0 1.0845021407222320E+02 1.0d0 1.0d0
532	2.0847323449769911E+02 1.0d0 1.0d0
533	4.0651541537167549E+02 1.0d0 1.0d0
534	8.0667634870078655E+02 1.0d0 1.0d0
536	3.3969004983391187E+03 1.0d0 1.0d0
537	7.2674336199173958E+03 1.0d0 1.0d0
538	1.6080864381912534E+04 1.0d0 1.0d0
539	3.6974131657844009E+04 1.0d0 1.0d0
541	2.2355921269411492E+05 1.0d0 1.0d0
542	5.9356338843429903E+05 1.0d0 1.0d0
543	1.6690413606262361E+06 1.0d0 1.0d0
544 545	4.9925104/26352403E+06 1.0d0 1.0d0 1.5952594555420512E+07 1.0d0 1.0d0
546	5.4660322670399554E+07 1.0d0 1.0d0
547	2.0153596325467077E+08 1.0d0 1.0d0
548	8.0207663178819859E+08 1.0d0 1.0d0
550	1.6143749848481022E+10 1.0d0 1.0d0
551	8.1990099053523590E+10 1.0d0 1.0d0
552	4.5329140391053540E+11 1.0d0 1.0d0
554	3.543348300000002E-02 1.0d0 1 0d0
555	6.5194588593144476E-02 1.0d0 1.0d0
556	1.1995577607433897E-01 1.0d0 1.0d0
557	2.2073349756341545E-01 1.0d0 1.0d0 4.0626019965028504E-01 1.0d0 1.0d0
559	7.4802874797813979E-01 1.0d0 1.0d0
560	1.3783189024559244E+00 1.0d0 1.0d0
561	2.5427420408376111E+00 1.0d0 1.0d0
562	4.6995778331749465E+00 1.0d0 1.0d0 8.7095624280738555E+00 1.0d0 1.0d0
564	1.6203216735620309E+01 1.0d0 1.0d0
565	3.0302909733749487E+01 1.0d0 1.0d0
566	5.7068235542655763E+01 1.0d0 1.0d0
568	2.0847323449769911E+02 1.0d0 1.0d0
569	4.0651541537167549E+02 1.0d0 1.0d0
570	8.0667634870078655E+02 1.0d0 1.0d0
571	1.6348107232313521E+03 1.0d0 1.0d0
573	7.2674336199173958E+03 1.0d0 1.0d0
574	1.6080864381912534E+04 1.0d0 1.0d0
575	3.6974131657844009E+04 1.0d0 1.0d0
$576 \\ 577$	8.8762049980994911E+04 1.0d0 1.0d0 2 2355921269411492E+05 1 0d0 1 0d0
578	5.9356338843429903E+05 1.0d0 1.0d0
579	1.6690413606262361E+06 1.0d0 1.0d0
580	4.9925104726352403E+06 1.0d0 1.0d0
100	1.000200420012ET0/ 1.000 1.000

1 1

582		5 4660322670399554E+07 1 0d0 1 0d0
583		2.0153596325467077E+08 1.0d0 1.0d0
584	30	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
585		3.543348300000002E-02 1.0d0 1.0d0
586		6.5194588593144476E-02 1.0d0 1.0d0
587		1.1995577607433897E-01 1.0d0 1.0d0
580		2.20/3349/56341545E-01 1.0d0 1.0d0
590		7 4802874797813979E-01 1 0d0 1 0d0
591		1.3783189024559244E+00 1.0d0 1.0d0
592		2.5427420408376111E+00 1.0d0 1.0d0
593		4.6995778331749465E+00 1.0d0 1.0d0
594		8.7095624280738555E+00 1.0d0 1.0d0
595		1.6203216735620309E+01 1.0d0 1.0d0
507		3.0302909/33/4948/E+01 1.0d0 1.0d0
598		1.0845021407222320E+02 1.0d0 1.0d0
599		2.0847323449769911E+02 1.0d0 1.0d0
600		4.0651541537167549E+02 1.0d0 1.0d0
601		8.0667634870078655E+02 1.0d0 1.0d0
602		1.6348107232313521E+03 1.0d0 1.0d0
603		3.3969004983391187E+03 1.0d0 1.0d0
605		1 6080864381912534E+04 1 0d0 1 0d0
606		3.6974131657844009E+04 1.0d0 1.0d0
607		8.8762049980994911E+04 1.0d0 1.0d0
608		2.2355921269411492E+05 1.0d0 1.0d0
609		5.9356338843429903E+05 1.0d0 1.0d0
610		1.6690413606262361E+06 1.0d0 1.0d0
612		4.9925104726352403E+06 1.0d0 1.0d0 1.5952594555420512E+07 1.0d0 1.0d0
613		5.4660322670399554E+07 1.0d0 1.0d0
614		2.0153596325467077E+08 1.0d0 1.0d0
615	25	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
616		3.543348300000002E-02 1.0d0 1.0d0
618		1.1995577607433897E-01 1.0d0 1.0d0
619		2.2073349756341545E-01 1.0d0 1.0d0
620		4.0626019965028504E-01 1.0d0 1.0d0
621		7.4802874797813979E-01 1.0d0 1.0d0
623		2 5427420408376111F+00 1 0d0 1 0d0
624		4.6995778331749465E+00 1.0d0 1.0d0
625		8.7095624280738555E+00 1.0d0 1.0d0
626		1.6203216735620309E+01 1.0d0 1.0d0
627		3.0302909733749487E+01 1.0d0 1.0d0
629		1 0845021407222320E+02 1 0d0 1 0d0
630		2.0847323449769911E+02 1.0d0 1.0d0
631		4.0651541537167549E+02 1.0d0 1.0d0
632		8.0667634870078655E+02 1.0d0 1.0d0
633		1.6348107232313521E+03 1.0d0 1.0d0
635		7 2674336199173958E+03 1 0d0 1 0d0
636		1.6080864381912534E+04 1.0d0 1.0d0
637		3.6974131657844009E+04 1.0d0 1.0d0
638		8.8762049980994911E+04 1.0d0 1.0d0
640		2.2355921269411492E+05 1.0d0 1.0d0 5.9356338843429903E+05 1.0d0 1.0d0
641	25	
642		3.543348300000002E-02 1.0d0 1.0d0
643		6.5194588593144476E-02 1.0d0 1.0d0
644		1.1995577607433897E-01 1.0d0 1.0d0
646		4.0626019965028504E-01 1.0d0 1.0d0
647		7.4802874797813979E-01 1.0d0 1.0d0
648		1.3783189024559244E+00 1.0d0 1.0d0
649		2.5427420408376111E+00 1.0d0 1.0d0
651		4.6995778331749465E+00 1.0d0 1.0d0 8.7095624280738555E+00 1.0d0 1.0d0
652		1.6203216735620309E+01 1.0d0 1.0d0
653		3.0302909733749487E+01 1.0d0 1.0d0
654		5.7068235542655763E+01 1.0d0 1.0d0
655		1.0845021407222320E+02 1.0d0 1.0d0
657		4 0651541537167549F+02 1 0d0 1 0d0
658		8.0667634870078655E+02 1.0d0 1.0d0
659		1.6348107232313521E+03 1.0d0 1.0d0
660		3.3969004983391187E+03 1.0d0 1.0d0
661		/.26/4336199173958E+03 1.0d0 1.0d0
663		3.6974131657844009E+04 1.0d0 1.0d0
664		8.8762049980994911E+04 1.0d0 1.0d0
665		2.2355921269411492E+05 1.0d0 1.0d0
666		5.9356338843429903E+05 1.0d0 1.0d0
007 668	20	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
669		6.5194588593144476E-02 1.0d0 1.0d0
670		1.1995577607433897E-01 1.0d0 1.0d0
671		2.2073349756341545E-01 1.0d0 1.0d0
672 672		4.0626019965028504E-01 1.0d0 1.0d0 7.4802874797813979E-01 1.0d0 1.0d0
010		1. TOV201T131013313E-01 1.000 1.000

674		1 37831890245592448+00 1 040 1 040
675		2 5427420408376111E+00 1 0d0 1 0d0
676		4.6995778331749465E+00 1.0d0 1.0d0
677		8.7095624280738555E+00 1.0d0 1.0d0
678		1.6203216735620309E+01 1.0d0 1.0d0
679		3.0302909733749487E+01 1.0d0 1.0d0
680		5.7068235542655763E+01 1.0d0 1.0d0
681		1.0845021407222320E+02 1.0d0 1.0d0
682		2.0847323449769911E+02 1.0d0 1.0d0
683		4.0651541537167549E+02 1.0d0 1.0d0
684		8.0667634870078655E+02 1.0d0 1.0d0
685		1.6348107232313521E+03 1.0d0 1.0d0
686		3.3969004983391187E+03 1.0d0 1.0d0
687		7.2674336199173958E+03 1.0d0 1.0d0
688	20	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
689		3.543348300000002E-02 1.0d0 1.0d0
690		6.5194588593144476E-02 1.0d0 1.0d0
691		1.1995577607433897E-01 1.0d0 1.0d0
692		2.2073349756341545E-01 1.0d0 1.0d0
693		4.0626019965028504E-01 1.0d0 1.0d0
694		7.4802874797813979E-01 1.0d0 1.0d0
695		1.3783189024559244E+00 1.0d0 1.0d0
696		2.5427420408376111E+00 1.0d0 1.0d0
697		4.6995778331749465E+00 1.0d0 1.0d0
698		8.7095624280738555E+00 1.0d0 1.0d0
699		1.6203216735620309E+01 1.0d0 1.0d0
700		3.0302909733749487E+01 1.0d0 1.0d0
701		5.7068235542655763E+01 1.0d0 1.0d0
702		1.0845021407222320E+02 1.0d0 1.0d0
703		2.0847323449769911E+02 1.0d0 1.0d0
704		4.0651541537167549E+02 1.0d0 1.0d0
705		8.0667634870078655E+02 1.0d0 1.0d0
706		1.6348107232313521E+03 1.0d0 1.0d0
707		3.3969004983391187E+03 1.0d0 1.0d0
708		7.2674336199173958E+03 1.0d0 1.0d0

1

Listing A.2: Output file for calculating the single point energy of Pb.

A.2 Optimizing a Basis Set for a Specific Electron Configuration

This input file will optimize a WTBS basis set for protactinium with a specific electron configuration. Note that in the output file, the "freeel" variable is set to 1. "freeel" only matters if "autogen" is set to true, the actual number of electrons in open shells is determined from the electron configurations that are read in.

1 91Pa 2 \$contrl jobtype='bsopt' \$end 3 \$nuc znuc=91 nucmdl=3 \$end 4 \$bas nsym=7 bastype='wtbs' \$end 5 \$tubs wtbspara-1.9453737E-02 1.8578241E+00 4.9471334E+00 1.4389341E+00 nbs=35 30 30 25 25 20 20 7 start=1 1 1 1 1 1 \$end 8 \$newuca rhobeg=1.0e-1 rhoend=1.0e-5 iprint=2 maxfun=2000 \$end 9 \$econfig nclose=7 5 5 3 3 1 1 nopen=0 0 0 1 1 1 1 nconf=6 \$end 10 0.0 0.0 0.1 0.0 0.0 2.0 11 0.0 0.0 0.0 1.0 0.0 2.0 12 0.0 0.0 0.0 1.0 0.0 2.0 13 0.0 0.0 0.0 1.0 0.0 2.0 14 0.0 0.0 0.0 1.0 2.0 0.0 15 0.0 0.0 0.0 1.0 2.0 0.0 16 \$scf maxitr=100 ixtrp=1 dfctr=0.5 \$end

Listing A.3: Input file for Pa basis set optimization calculation.



14	NGROUP = 1
15	
16	&WTBS
17	WTESPARA = 1.945373699999999999-002,
18	1.85782410000000 ,
19	4.94/13340000000 , 1.4389410000000
20	NRS = 35.
22	30,
23	30,
24	25,
25	25,
26	20,
27	20, START = 1
29	1,
30	1,
31	1,
32	1,
33	1,
35	GROUPS = 1.
36	1,
37	1,
38	1,
39	1,
40	1,
41 49	
43	enewuoa
44	RHDBEG = 0.10000000000000 ,
45	RHDEND = 1.0000000000001E-005,
46	IPRINT = 2,
47	MAXFUN = 2000
40	AFCONFIG
50	NCLOSE = 7,
51	5,
52	5,
53	3,
54	3,
56	1,
57	NOPEN = 0,
58	0,
59	0,
60	1,
62	1, 1
63	· , 1,
64	FREEL = 1,
65	AUTOGEN = F,
66	NCONF = 6
68	/ nconf = 6
69	1 0.00 0.00 1.00 0.00 1.00 0.00 2.00
70	2 0.00 0.00 0.00 1.00 0.00 1.00 1.00
71	3 0.00 0.00 1.00 0.00 2.00 0.00
72	4 0.00 0.00 0.00 1.00 1.00 0.00 2.00
74	
75	SSCF
76	MAXITR = 100,
77	IXTRP = 1,
78	DFCTR = 0.5000000000000 ,
79	INDL = 1.000000000000001E-005, THRE = 0.0000000000000000000000000000000000
81	THDS = 1.0000000000001E-009
82	
83	31560
84	166068720
85	82680
87	221424960
88	Calculating one electron integrals
89	Calculating two electron integrals
90	Calculating guess
91	Starting SUF
93	on converse as relation on limit energy - 21514-01010000040
94	
95	1S+ 2S+ 3S+ 4S+ 5S+ 6S+ 7S+
96	-4.1678558E+03 -7.8202807E+02 -1.9970550E+02 -5.2156121E+01 -1.1997891E+01 -2.0501109E+00 -1.9881466E-01
97	
99	1.9453737E-02 4.5526064E-07 6.1600046E-06 -6.1423490E-05 4.8451991E-05 -1.0511245E-04 1.3158903E-04 -1.8724908R-01
100	3.6141658E-02 -1.9479713E-06 -2.6351782E-05 2.6251028E-04 -2.0608864E-04 4.3702976E-04 -4.8933088E-04 -5.0769082E-01
101	6.7145353E-02 4.6364451E-06 6.2698403E-05 -6.2360865E-04 4.8527658E-04 -9.8904771E-04 2.4811733E-03 -4.9371359E-01
102	1.2474818E-01 -8.4540743E-06 -1.1426442E-04 1.1332041E-03 -8.7060948E-04 1.6324965E-03 1.8661239E-02 -1.0195880E-01
103	2.01102112 01 1.0300/#312/00 1.01050012/04 1.10510092/05 1.32104012/05 2.04409302/05 2.10531992/01 2.0423062/01 4.3071102/01 1.9941795E-05 -2.6910468E-04 2.63110827E-03 1.976407E-03 1.089307E-03 7.8864637E-01 4.500904E-01
105	8.0055661E-01 2.8321063E-05 3.8110568E-04 -3.7093835E-03 2.3287542E-03 -3.6107270E-02 5.0398773E-01 2.2648026E-01
1	

106	1.4887931E+00	-3.9289907E-05	-5.2704055E-04	5.0770781E-03	-1.9095251E-03	-4.6247606E-01	-6.1984690E-01	-2.3106351E-01
107	2.7707233E+00	5.4127358E-05	7.3096927E-04	-6.5063021E-03	1.0470406E-02	-1.0705943E+00	-9.6963877E-01	-3.4091033E-01
108	5 1625848E+00	-7 1730547E-05	-9 5665668E-04	8 5020340E-03	2 3278340F-01	1 22/8776E-01	4 3766720F-02	1 53566818-02
100	5.10250406.00	1.11303416 03	3.3003000E 04	0.3020340E 03	2.32/03405 01	1.22407705 01	4.51001206 02	1.0000016 02
109	9.6361639E+00	9.2150385E-05	1.1905804E-03	-1.4907331E-02	9.8537025E-01	1.2755242E+00	7.2196144E-01	2.2937092E-01
110	1.8031447E+01	-1.2623899E-04	-1.7792297E-03	-1.1538348E-01	3.8510740E-01	3.3727265E-01	1.7145582E-01	5.4245805E-02
111	3.3858337E+01	1.5373486E-04	2.6018880E-03	-6.9733818E-01	-9.8256369E-01	-6.2697726E-01	-2.9682747E-01	-9.2176854E-02
110	6 38756005101	1 15257405 04	2 80035405 00	6 0473604E 01	6 4464017E 01	2 01050605 01	1 0064601E 01	E ECOE7COE 00
114	0.30/30926-01	-1.1555749E-04	3.0093340E-02	-0.04/30046-01	-0.440491/E-01	-3.9120006-01	-1.0004021E-01	-3.3003703E-02
113	1.2125177E+02	1.2587653E-04	3.1220205E-01	3.3102664E-01	2.2711991E-01	1.2336342E-01	5.5360335E-02	1.6941375E-02
114	2.3200920E+02	-1.4331244E-03	5.2657623E-01	5.2989905E-01	3.2983813E-01	1.6974036E-01	7.5889627E-02	2.3305591E-02
115	4 4845175E+02	-3.5900271E-02	2.6241533E-01	2.1315943E-01	1.2658256E-01	6.4910423E-02	2.8848768E-02	8.8309114E-03
116	0.770100000000	1 60070055 01	E 4277100E 00	0 1040101 00	1 05676545 00	E 0701006E 02	0.00045605.02	6 07025705 04
110	0.//01009E+02	-1.6237035E-01	-5.4377160E-02	-2.1340131E-02	-1.050/054E-02	-5.2701266E-03	-2.2994560E-03	-0.9/935/6E-04
117	1.7450942E+03	-2.6616678E-01	-1.5722966E-01	-8.1885030E-02	-4.2968044E-02	-2.1145552E-02	-9.3451415E-03	-2.8633384E-03
118	3.5348455E+03	-2.5104786E-01	-1.3570153E-01	-6.9567552E-02	-3.6553325E-02	-1.8070096E-02	-7.9768505E-03	-2.4411779E-03
119	7 3220404F+03	-1 7657870F-01	-8 7651162F-02	-4 4131448F-02	-2 3016579F-02	-1 1330730F-02	-5 0026903E-03	-1 5318434F-03
100	1 55714525104	1.00000700 01	E 0277626E 00	0 F120416E 00	1 2002000E 02	6 45646105 02	0.002000000 00	0.7010260E 04
120	1.55/14536+04	-1.00995/2E-01	-5.03//636E-02	-2.51304166-02	-1.3036300E-02	-0.4504012E-05	-2.04931196-03	-0.72103606-04
121	3.4144729E+04	-6.0291269E-02	-2.7398442E-02	-1.3574384E-02	-7.0546649E-03	-3.4711606E-03	-1.5320152E-03	-4.6902952E-04
122	7.7552073E+04	-3.2990939E-02	-1.4620144E-02	-7.2147644E-03	-3.7489374E-03	-1.8457668E-03	-8.1446829E-04	-2.4930193E-04
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194	4 53100025105	0 50000175 02	4 10105105 00	0.0110217E 02	1 04250055 02	E 1340000E 04	0.06570105.04	6 02520115 05
124	4.5516623E+05	-9.5990017E-03	-4.1016510E-03	-2.0116317E-03	-1.0435965E-03	-5.1349929E-04	-2.205/310E-04	-0.9353611E-05
125	1.1774969E+06	-5.0914462E-03	-2.1481685E-03	-1.0512710E-03	-5.4487705E-04	-2.6798839E-04	-1.1824674E-04	-3.619/166E-05
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127	9.4102964E+06	-1.3140471E-03	-5.4552441E-04	-2.6624977E-04	-1.3791178E-04	-6.7820854E-05	-2.9923603E-05	-9.1599121E-06
1.9.9	0.0016900E+07	-6 0000997E-04	-2 52021005-04	-1 00015965-04	-6 2660006E-0E	-2 1200E72E-0E	_1 20120/1E_0E	-4 0004407E-06
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129	9.7128202E+07	-1.6932067E-04	-6.9765935E-05	-3.4006601E-05	-1.7609042E-05	-8.6588446E-06	-3.8203370E-06	-1.1694392E-06
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122	E E067200E+00	0 06674005-09	2 000000212 01	1 0612206E-00	0 60452005-00	A 70E9261E_00	0.000000000	6 20E0E21E_10
102	0.000/302E+09	J.2001492E-08	5.02025U3E-08	1.0010390E-08	0.0240329E-09	1200301E-09	2.0000200E-09	0.3000531E-10
133	2.5314129E+10	-1.2866632E-08	-5.3038951E-09	-2.5841696E-09	-1.3361905E-09	-6.5608747E-10	-2.8953396E-10	-8.8655105E-11
134								
135								
136	1 0/537275-00	-F 0363704E-00	1 18162445-00	-7 11300745-00	3 26260075-00	-1 01010645-07	1 10054045-07	-1 65052175-04
107	1.3400/0/E-02	J.U303/U0E-09	1010344E-09	1.11302/4E-08	0.2020991E-08	1.0191204E-07	1.10000046-07	1.0000001/E-04
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140	0.2170017E 01	0.22110040 00	E 0161101E 07	E 0004200E 00	2 0006202E 06	7 25620015 06	9.3761000E 04	0.05450405.04
140	2.31/021/E-01	-0.5290474E-06	5.3101101E-07	-2.0924309E-00	3.0006303E-06	-/.3503901E-00	0.3/01902E-04	0.95452466-04
141	4.3071120E-01	1.0208035E-07	-1.0912541E-06	1.1564757E-05	-7.6428230E-06	4.9288760E-06	3.2706490E-03	1.8751516E-03
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1.4.5	2.1101233E+00	0.0200709E-00	1.1091835E-00	-7.0519162E-05	1.0910313E-04	-1.12041276-02	-1.01994936-02	-3.3636403E-03
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1.40	0.0000001101	1.2024024E 00	4 00040505 00	2.01002428 02	0.010000000 02	4.00404000 02	0.050500000 00	0.0000000000000000000000000000000000000
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1 2 0			1100012022 00					
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$150 \\ 151$	1.2125177E+02 2.3200920E+02	6.0105809E-06 -1.4693522E-04	2.2053270E-02 5.0989297E-02	2.3275860E-02 5.0595306E-02	1.5984258E-02 3.1409317E-02	8.6821874E-03 1.6152076E-02	3.8967421E-03 7.2202503E-03	1.1925690E-03 2.2172770E-03
$150 \\ 151 \\ 152$	1.2125177E+02 2.3200920E+02 4.4845175E+02	6.0105809E-06 -1.4693522E-04 -5.3310399E-03	2.2053270E-02 5.0989297E-02 3.4317940E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03
150 151 152	1.2125177E+02 2.3200920E+02 4.4845175E+02	6.0105809E-06 -1.4693522E-04 -5.3310399E-03	2.2053270E-02 5.0989297E-02 3.4317940E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03
$150 \\ 151 \\ 152 \\ 153$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04
150 151 152 153 154	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04
150 151 152 153 154 155	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04
150 151 152 153 154 155 156	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404F+03	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.056359E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04
150 151 152 153 154 155 156	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571452E+04	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.0234772E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.0506359E-02 2.027611E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4072564E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.792300E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03 -2.8340379E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.601472E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -5.172708E-04
150 151 152 153 154 155 156 157	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03 -3.8340378E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -5.1773708E-04
150 151 152 153 154 155 156 157 158	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -4.9557458E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03	$\begin{array}{c} 8.6821874E-03\\ 1.6152076E-02\\ 8.3130239E-03\\ -1.2082964E-03\\ -5.4284824E-03\\ -6.1904548E-03\\ -5.1518739E-03\\ -3.8340378E-03\\ -2.6224758E-03\\ \end{array}$	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -1.6916478E-03 -1.1572758E-03	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -5.1773708E-04 -3.5430612E-04
150 151 152 153 154 155 156 157 158 159	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -4.9557458E-02 -3.2965670E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03	1.5984258E-02 3.1409317E-02 1.6222173E-02 2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -3.8340378E-03 -2.6224768E-03 -1.7203202E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.608834E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -5.1777708E-04 -3.5433612E-04 -2.3230106E-04
150 151 152 153 154 155 156 157 158 159 160	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.322040E+03 1.5571453E+04 3.4144729E+04 1.833176E+05	6.0105809E-06 -1.4693522E-04 -5.3310399E-03 -3.3138881E-02 -7.4346622E-02 -8.8657364E-02 -8.8657364E-02 -6.9734773E-02 -4.9557458E-02 -3.2965670E-02 -2.0881919E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -8.6643540E-03	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-03 -2.1893129E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7762022E-03 -1.0762097E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 4.748654E-04	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6083394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -5.1773708E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04
150 151 152 153 154 155 156 157 158 159 160 161	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.531827E-05	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -4.9557458E-02 -3.2965670E-02 -2.0881919E-02 -1.266964E-02	2.2053270E-02 5.0989297E-02 -1.1199777E-02 -4.7725194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -8.6643540E-03 -5.2369607E-03	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03 -4.226426E-03 -2.56426E-03	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-03 -2.1893129E-03 -1.322908E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7762097E-03 -6.5117137E-04	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3982415E-03 -2.7322183E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486954E-04	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -5.1773708E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 8.792952E-05
150 151 152 153 154 155 156 157 158 159 160 161 162	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 4.8331766E+05 4.531766E+05	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.865736E-02 -6.9734773E-02 -4.9557458E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03	2.3275860E-02 5.0595306E-02 2.7410766E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.02529869E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-03 -2.1883129E-03 -1.326088E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.77203202E-03 -1.0762097E-03 -6.5117130E-04	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904465E-04 -2.3988415E-03 -2.7322183E-03 -2.7322182E-03 -1.6916478E-03 -1.6916478E-03 -1.572758E-03 -7.5897747E-04 -4.7466554E-04	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.793253E-05
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.833176E+05 4.531823E+05 1.1774969E+06	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-02 -7.3479864E-03	2.2053270E-02 5.0989297E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03 -4.2262845E-03 -1.4766257E-03	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -3.34955699E-03 -2.1893129E-03 -1.3226088E-03 -7.6444915E-04	8.6821874E-03 1.6152076E-02 8.313029E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224768E-03 -1.7203202E-03 -1.0762097E-03 -6.5117130E-04 -3.7581084E-04	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3928415E-03 -2.7322183E-03 -2.7322183E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 -2.872842E-04 -1.6581658E-04	$\begin{array}{c} 1.1925690E{-}03\\ 2.2172770E{-}03\\ 1.1306051E{-}03\\ -1.6088394E{-}04\\ -7.3499143E{-}04\\ -8.3610751E{-}04\\ -8.3610751E{-}04\\ -6.9638073E{-}04\\ -5.1773708E{-}04\\ -3.5430612E{-}04\\ -2.3230106E{-}04\\ -1.4537414E{-}04\\ -8.793253E{-}05\\ -5.0760481E{-}05\\ \end{array}$
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 1.8331766E+05 4.5318823E+05 1.1774969E+06 3.2312830E+06	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -3.2965670E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03	2.3275860E-02 5.0595306E-02 2.741076E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03 -1.4766257E-03 -8.0945657E-04	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.702027E-03 -6.5117130E-04 -3.7581084E-04 -2.0623615E-04	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904465E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.592747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.7932535E-05 5.0760481E-05 -2.7850367E-05
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 1.1774969E+06 3.2312890E+06 9.410296E+06	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -1.2669461E-02 -1.2669461E-02 -2.0258641E-03 -2.0258641E-03	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -1.3787754E-02 -5.2369602E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.307837E-02 -2.307837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.546257E-03 -1.4766257E-03 -8.0945657E-04 -4.0601852E-04	1.5994258E-02 3.1409317E-02 2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-02 -1.3236088E-03 -1.3236088E-03 -7.644915E-04 -4.1927555E-04 -2.1018983E-04	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.0762097E-03 -1.0762097E-03 -6.5117130E-04 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -1.6916478E-03 -1.6916478E-03 -7.5897747E-04 -4.748654E-04 -2.8728442E-04 -1.6581658E-04 9.0988010E-05 -4.5593595E-05	1.1325690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -5.1773708E-04 -3.5430612E-04 -2.3230106E-04 -8.732532E-05 -5.0760481E-05 -2.7850367E-05 -1.3957078E-05
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.833176E+05 4.5318823E+05 3.2312890E+06 9.4102964E+06 9.4102964E+06	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -3.29557458E-02 -3.2955670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.084541E-03 -8.4844613E-04	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.326185E-04 -3.4885394E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03 -1.4766257E-03 -8.0945657E-04 -4.0601852E-04	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -2.1018983E-04 -8.8049493E-05	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.70762097E-03 -3.7581084E-04 -2.0623615E-04 -1.333653E-04 -4.330688E-05	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.398415E-03 2.7322183E-03 -2.7322183E-03 -2.7242441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.7932535E-05 -5.0760481E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 1.1774969E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07	6.0105809E-06 -1.4693522E-04 -5.3310398-03 -7.4346622E-02 -9.4791276E-02 -8.865736E-02 -8.865736E-02 -8.865736E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-02 -7.3479864E-03 -2.0258641E-03 -8.484513E-04 -1.51072E-04	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.506359E-02 -3.0375011E-02 -2.1009571E-02 -3.643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -3.4885394E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-03 -1.4766257E-03 -8.0945657E-04 -4.0601852E-04 -1.700036E-04	1.5994258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -7.7832300E-03 -5.3347565E-03 -2.1883129E-03 -2.1883129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -2.1018983E-04 -8.8049433E-05	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.0762097E-03 -6.5117130E-04 -3.7581084E-04 -2.6623615E-04 -1.0333633E-04 -4.3308889E-05 -2.60266E-06	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486554E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6083394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-04 -8.739253E-05 -2.760481E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.833176E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -8.4844613E-04 -1.5105779E-04 4.1505779E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.505778E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04 -1.50578E-04	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.4273564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-04 -4.0601852E-04 -1.7000306E-04 -3.0252716E-05	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -7.7832300E-03 -3.4955699E-03 -3.4955699E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -8.8049493E-05 -1.5655586E-05	8.6821874E-03 1.6152076E-02 8.313029E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -1.033633E-04 -4.3308889E-05 -7.6940850E-06 -7.6940850E-06	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3982415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.6516478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486554E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06	1.1306051E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.7932535E-05 -5.0760481E-06 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 -1.039342E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0393442E-06 -1.0395448-08 -1.0395448-08 -1.0395448-08 -1.0395448-08 -1.0395448-08 -1.0395448-08 -1.0395448-08 -1.0395448-08 -1.0395448-08 -1.039548
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 3.4144729E+04 1.8331766E+05 4.531832B+05 1.1774969E+06 3.2312830E+06 9.4102964E+06 2.9212830E+07 3.4711732E+08	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -8.8657364E-02 -8.8657364E-02 -8.9557458E-02 -3.2965670E-02 -3.2965670E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -8.4844613E-04 -1.5105779E-04 1.704689E-05	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.07025194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06	2.3275860E-02 5.0595306E-02 2.7410766E-02 -2.7410766E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.0294910E-02 -1.4973564FE-03 -4.2282845E-03 -2.5546250E-03 -8.0945657E-04 -1.4766257E-04 -1.4061852E-04 -3.0252716E-05 2.3357655E-06	$\begin{array}{c} 1.5984258E-02\\ 3.1409317E-02\\ 1.6222173E-02\\ -2.4170697E-03\\ -1.1035434E-02\\ -1.2529869E-02\\ -1.2529869E-02\\ -1.0475076E-02\\ -7.7832300E-03\\ -5.3347585E-03\\ -3.4955699E-03\\ -2.1893129E-03\\ -1.3236088E-03\\ -3.4955699E-03\\ -1.3236088E-04\\ -4.1927555E-04\\ -2.1018983E-04\\ -8.8049493E-05\\ -1.5655568E-05\\ -1.5655568E-05\\ -1.2056324E-06\\ \end{array}$	$\begin{array}{c} 8.6821874E-03\\ 1.6152076E-02\\ 8.3130239E-03\\ -1.2082964E-03\\ -5.4284824E-03\\ -5.151873E-03\\ -3.8340378E-03\\ -2.6224758E-03\\ -1.7203202E-03\\ -1.7203202E-03\\ -1.7203202E-03\\ -1.7261084E-04\\ -2.0623615E-04\\ -1.0333633E-04\\ -4.330889E-05\\ -7.6940850E-06\\ 5.9103384E-07\end{array}$	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904465E-04 -2.3988415E-03 -1.6916478E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 -4.786654E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 2.3949229E-06 2.6088264E-07	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -1.4537414E-04 -8.7932535E-05 -5.0760481E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06 7.9906891E-08
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 3.534845E+03 7.3220404E+03 3.534845E+03 3.4144729E+04 7.7552073E+04 1.833176E+05 3.231280E+06 9.4102964E+06 2.9216992E+07 9.712802E+07 3.4711732E+08 1.3384720E+09	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.2965670E-02 -3.2965670E-02 -7.3479864E-03 -1.2669461E-02 -7.3479864E-03 -2.0258641E-03 -2.0258641E-04 -1.5105779E-04 1.1704689E-05 -3.9489441E-06	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -3.6292815E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-03 -2.554250E-03 -8.0945657E-04 -1.7000306E-04 -3.052716E-05 2.3357655E-06 -7.8782411E-07	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -8.8049493E-05 -1.565586E-05 1.2056324E-06 -4.0646724E-07	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -6.5117130E-04 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.398415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.6516478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486554E-04 -2.78842E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06	1.1305690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.4537414E-05 -2.7850367E-05 -3.8484891E-06 -1.0393242E-06 -7.9906891E-08 -2.632237E-08
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 3.2312890E+06 9.4102964E+06 2.9216892E+07 3.4714732E+08 1.3384720E+09 5.5867332E+09	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8557364E-02 -4.9557458E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.0288641E-03 -3.9489441E-04 1.5105779E-04 1.1704689E-05 -3.9489441E-06 1.3761821E-06	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -3.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3226185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435596E-07	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03 -1.4766257E-03 -1.4766257E-04 -4.0601852E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07	$\begin{array}{c} 1.5984258E-02\\ 3.1409317E-02\\ 1.6222173E-02\\ -2.4170697E-03\\ -1.035434E-02\\ -1.2529869E-02\\ -1.2529869E-02\\ -7.782300E-03\\ -5.3347585E-03\\ -3.4955699E-03\\ -2.1893129E-03\\ -1.3236088E-03\\ -1.3236088E-03\\ -1.3236088E-03\\ -1.41927555E-04\\ -2.1018983E-04\\ -2.1018983E-05\\ -1.5655568E-05\\ -1.2056324E-06\\ -4.0646724E-07\\ -4.412013E-07\\ -1.4162013E-07\\ \end{array}$	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04 -1.3336838E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 -6.9388206E-08	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.398415E-03 -2.2742241E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-03 -8.3610751E-04 -8.3610751E-04 -2.3230106E-04 -1.4537414E-04 -8.793253E-05 -5.0760481E-05 -5.3760481E-06 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 2.6932237E-08 9.3829787E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 3.4144729E+04 4.531823E+05 1.1774969E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 9.7128202E+07 9.7128202E+07 9.534120E+09 5.5867382E+09	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 -1.1704698E-05 -3.9489441E-06 1.3761821E-06 -3.9881448E-07	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -5.2369602E-03 -3.0292815E-03 -1.6660611E-03 8.432945E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6356484E-07	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.300783E-02 -2.300783E-02 -2.147306E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -4.2282845E-03 -2.554250E-03 -2.554250E-03 -3.045657E-04 -1.7000306E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.955325E-08	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -7.7832300E-03 -3.4955699E-03 -3.4955699E-03 -2.1893129E-03 -7.6444915E-04 -4.1927555E-04 -8.8049493E-05 -1.5655586E-05 -1.2056324E-06 -4.0646724E-07 1.4162013E-07 -4.10389E-08	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -6.5117130E-04 -3.7581084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 2.0107018E-08	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.1572758E-03 -1.1572758E-03 -7.5897747E-04 -4.7486954E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 8.875999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6083394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -8.361073E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.739253E-05 -5.0760481E-05 -2.7880367E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.990681E-08 -2.6932237E-08 9.3829787E-09 -2.718978F-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 171\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 4.5418823E+05 4.5318823E+05 3.2312890E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -4.0327779E-04 1.5105779E-04 1.5105779E-04 1.3761821E-06 -3.9881449E-07	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3226185E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.390783TE-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03 -1.4766257E-03 -8.0945657E-04 -3.0252716E-05 2.3357655E-06 7.3782411E-07 2.7452198E-07 -7.9553252E-08	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -2.1018983E-04 -8.8049493E-05 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 1.4162013E-07 -4.1038958E-08	8.6821874E-03 1.6152076E-02 8.313029E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -6.1904548E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -0.5117130E-04 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04 -4.330889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 -1.9917466E-07 -1.9917466E-07 -1.9917466E-07 -1.9917466E-07 -2.0107018E-08	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.7322183E-03 -2.742441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.7932535E-05 -5.0760481E-05 -2.7850367E-05 -1.3957078E-05 -5.8484881E-06 -1.0393242E-06 7.9906881E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.2965670E-02 -3.2965670E-02 -7.3479864E-03 -1.266949E1-02 -7.3479864E-03 -0.0258641E-03 -8.4844613E-04 -1.5105779E-04 1.1704689E-05 -3.9489441E-06 1.3761821E-06 -3.9881149E-07	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0705194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -3.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -1.0294910E-02 -6.7413567E-03 -4.2202845E-03 -1.4766257E-03 -2.554625E-03 -3.0945657E-04 -1.7000306E-04 -3.0525716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08	1.5994258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -2.1018983E-04 -8.8049493E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.726304E-04 -2.0623615E-04 -1.0333633E-04 -4.330889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904465E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486554E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 2.3394929E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1306051E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-04 -1.4537414E-04 -8.793253E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7761809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.32965670E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -8.4844618E-04 -1.5105779E-04 1.1704689E-05 -3.9489441E-06 1.3761821E-06 -3.9881149E-07	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6666011E-03 -8.3326185E-04 -6.2100174E-05 4.8007844E-06 5.6435969E-07 -1.63521E-06 5.6435969E-07 -1.6354648E-07	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.4973564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03 -1.4766257E-04 -4.0601852E-04 -1.7000306E-04 -3.0252716E-05 2.3357655E-05 -7.8782411E-07 2.7452198E-07 -7.9553252E-08	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -1.2529869E-03 -3.4955699E-03 -3.4955699E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -8.804493E-05 -1.5655586E-05 1.2056324E-05 -1.5655586E-05 -1.265328E-04 -4.0646724E-07 1.4162013E-07 -4.1038958E-08	8.6821874E-03 1.6152076E-02 8.313029E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -3.8340378E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -3.7581084E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 -6.9388206E-08 -2.0107018E-08	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.27322183E-03 -2.2742441E-03 -1.6916478E-03 -7.5897747E-04 -4.7486954E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1306051E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 1.1774969E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.3138881E-02 -7.4346622E-02 -8.8657364E-02 -8.8557364E-02 -8.957458E-02 -3.2965670E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.028841E-04 -1.5105779E-04 1.1704689E-05 -3.9889441E-06 -3.9881149E-07 2P-	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.775194E-02 -4.7754793E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787764E-02 -8.6643540E-03 -5.2369602E-03 -1.3685504 -3.292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07	2.3275860E-02 5.0595306E-02 2.741076E-02 -2.741076E-02 -2.3907837E-02 -2.0147306E-02 -1.4973564E-02 -1.4973564E-02 -1.4924910E-02 -6.7413567E-03 -2.5546250E-03 -2.5546250E-03 -1.4766257E-04 -4.0601852E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 -7.9553252E-08	1.5994258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.34955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -2.1018983E-04 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -6.5117130E-04 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04 -7.6340850E-06 5.9103384E-07 -1.9917466E-07 -6.9388206E-08 -2.0107018E-08	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904465E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.59774E-04 -4.7486954E-04 -2.8728442E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-04 -8.793253E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 -2.6332237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174 \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 3.534845E+03 7.3220404E+03 3.534845E+04 7.7552073E+04 7.7552073E+04 1.8331766E+05 3.231280E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -1.2669461E-02 -7.3479664E-03 -2.0258641E-03 -8.4844613E-04 -1.5105779E-04 1.1704689E-05 -3.9489141E-06 -3.9481149E-07 -7.5278375E+02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -5.2369602E-03 -3.0292815E-03 -1.6060111E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07 -1.6354648E-07	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-04 -2.5546250E-03 -8.0945657E-04 -1.700306E-04 -3.052716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -7.7832300E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -8.8049493E-05 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -3.36381084E-07 -1.9317466E-07 6.3388206E-08 -2.0107018E-08 -2.0107018E-08 -1.2849029E+00	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.6516478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486554E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -3.5430612E-04 -5.0760481E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 -2.0392237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 173\\ 174\\ 175\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.531823E+05 1.1774969E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 9.5384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8557364E-02 -4.9557458E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.028841E-03 -3.9489441E-04 1.5105779E-04 1.1704689E-05 -3.9489441E-06 -3.9881149E-07 -7.5278375E+02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0705194E-02 -4.070539E-02 -3.0375011E-02 -2.1009571E-02 -8.6643540E-03 -5.2369602E-03 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.64355969E-07 -1.6354648E-07	2.3275860E-02 5.0595306E-02 2.741076E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.0147306E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03 -1.4766257E-03 -1.4766257E-04 -4.0601852E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08	1.5994258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.64449145E-04 -4.1927555E-04 -2.1018983E-04 -1.5655586E-05 1.2655586E-05 1.2655586E-05 1.2655586E-05 1.2655586E-05 1.2655586E-05 1.2655586E-05 1.2655284E-06 -4.0646724E-07 -4.1038958E-08	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-04 -2.0623615E-04 -1.3336838E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 -6.9388266E-08 -2.0107018E-08 -2.0107018E-08	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904465E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6516478E-03 -1.1572758E-03 -7.589774E-04 -4.7486954E-04 -2.8728442E-04 -9.0988010E-05 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-03 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.793253E-05 -5.0760481E-05 -5.0760481E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 -2.6932237E-08 9.3829787E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 155\\ 156\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 3.2312890E+06 3.2312890E+06 2.9216892E+07 9.410294E+06 2.9216892E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.025864E-03 -2.025864E-03 -3.249864E-04 -1.5105779E-04 1.1704689E-05 -3.9489141E-06 -3.9489141E-07 2P- -7.5278375E+02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6355421E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.24766257E-03 -2.554250E-03 -2.554250E-03 -1.4766257E-04 -4.0601852E-04 -1.7000306E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -3.4955699E-03 -3.4955699E-03 -2.1893129E-03 -3.4955699E-03 -7.6444915E-04 -4.1927555E-04 -4.1927555E-04 -8.8049493E-05 -1.5655586E-05 -1.5655582E-05 -1.6665724E-07 -4.1038958E-08 -9.6061333E+00	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -6.5117130E-04 -3.7561084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.1572758E-03 -1.1572758E-03 -7.5897747E-04 -4.7486954E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.357078E-05 -2.7850367E-05 -5.8484891E-06 -1.0393242E-06 -1.0393242E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 176\\ 176\\ 176\\ 176\\ 176\\ 176\\ 176$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -3.9489441E-06 -3.9489441E-06 -3.9489441E-06 -3.9489141E-06 -3.9881149E-07 -7.5278375E+02 -0.00000000000000000000000000000000000	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -3.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3226185E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02 -1.8645886E+02	2.3275860E-02 5.0595306E-02 2.741076E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.5546250E-03 -1.4766257E-04 -4.0601852E-04 -3.0252716E-05 2.3357655E-06 7.7.8782411E-07 -7.8782411E-07 -7.9553252E-08 4P- -4.6168113E+01	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.64449145E-04 -4.1927555E-04 -2.1018983E-04 -2.1018983E-05 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08 -4.1038958E-08 -5P- -9.6061333E+00	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04 -1.3033632E-04 -1.9917466E-07 -6.9388206E-08 -2.0107018E-08 -2.0107018E-08 -1.2849029E+00 -2.00005	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.27322183E-03 -2.2742441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-05 -5.0760481E-05 -5.0760481E-05 -5.8484881E-06 -1.0393242E-06 7.9906881E-08 -2.6932237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 3.4144729E+04 6.531823E+05 1.1774969E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 9.7128202E+07 9.5312420E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 1.1704698E-05 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -2.5278375E+02 9.0965057E-07	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -3.0292815E-03 -1.6606011E-03 -8.326168E-04 -3.4885394E-04 -6.2100174E-05 5.435969E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -1.0294910E-02 -1.0294910E-02 -1.2292040E-03 -1.2262462E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -2.3547655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 4P- -4.6168113E+01 -4.3994948E-05	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.6222173E-02 -2.4170697E-03 -1.529869E-02 -1.2529869E-02 -3.4955699E-03 -3.4955699E-03 -2.1893129E-03 -7.6444915E-04 -4.1927555E-04 -3.8049493E-05 -1.565586E-03 -1.265538E-06 -4.0646724E-07 1.4162013E-07 -4.1038958E-08 -5P- -9.6061333E+00 -2.0416597E-05	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -5.517130E-04 -3.7581084E-04 -2.0623615E-04 -4.330889E-05 -7.6940850E-06 -3.940850E-06 -2.0107018E-08 -2.0107018E-08 -2.0107018E-08 -2.6310064E-04 -2.6310064E-04	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -7.5897747E-04 -1.1572758E-03 -7.5897747E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 3.0630487E-08 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.3957078E-05 -2.7850367E-05 -3.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.0393242E-09 -2.6932237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 177\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 4.531823E+05 4.531823E+05 9.4102964E+06 2.9216892E+07 9.4102964E+06 2.9216892E+07 9.411732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.329565705E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -2.0258641E-03 -3.9489441E-06 -3.9489441E-06 -3.9489441E-06 -3.9489441E-06 -3.9489441E-06 -3.9489441E-06 -3.9881149E-07 -7.5278375E+02 9.0965057E-07 -3.5075358E-06	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3226185E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05	2.3275860E-02 5.0595306E-02 2.7410765E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-04 -1.4766257E-04 -1.40601852E-04 -1.7000306E-04 -3.0252716E-05 2.3357655E-06 2.3357655E-06 7.3782411E-07 -7.3752312E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.2529869E-03 -5.3347585E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -2.1018983E-04 -2.1018983E-05 -1.5655586E-05 1.2056324E-06 -1.5655586E-05 1.2056324E-06 -1.4162013E-07 -4.1038958E-08 -9.6061333E+00 -2.0416597E-05 7.1672253E-05	8.6821874E-03 1.6152076E-02 8.313029E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -6.1904548E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -3.7581084E-04 -2.0623615E-04 -1.0333632E-04 -1.0333632E-04 -3.7581084E-07 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.7322183E-03 -2.742441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-04 -3.5430106E-04 -1.4537414E-04 -2.3230106E-05 -5.0760481E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-07	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -3.2965670E-02 -7.0881919E-02 -7.0881919E-02 -7.3479864E-03 -4.0527727E-03 -8.4844613E-04 -1.5105779E-04 1.1704698E-05 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -7.5278375E+02 9.0965057E-07 -3.5075358E-06	2.2053270E-02 5.0989297E-02 5.0989297E-02 1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -5.2369602E-03 -1.66606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 5.435965E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 -4.9695762E-05 -4.9695762E-05 -4.9695762E-05 -4.9695762E-05 -4.9	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.300783T-02 -2.300783T-02 -2.147306E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -4.2282845E-03 -2.554250E-03 -2.554250E-03 -3.05675E-04 -3.052716E-05 -3.357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 4P- -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.750775F-04	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.2529869E-03 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -1.3226088E-03 -7.6444915E-04 -4.192755E-04 -4.192755E-04 -2.1018982E-04 -2.1018982E-04 -1.265586E-05 -1.565586E-05 -1.565586E-05 -1.665582E-06 -4.0646724E-07 1.4162013E-07 -4.1038958E-08 -9.6061333E+00 -2.0416597E-05 7.1672253E-05 -2.053537E-04	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -6.5117130E-04 -3.7581084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.0107018E-08 -2.6310064E-04 -5.6527666E-05 -6.1665581E-03	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -7.5897747E-04 -1.1572758E-03 -7.5897747E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 3.0630487E-08 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.357078E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.930581E-08 -2.6932237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7761809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 7.7552073E+04 1.83176E+05 3.231280E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 4.7145353E-02	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 1.3761821E-06 -3.9881149E-07 -3.988149E-07 -3.5278375E+02 9.0965057E-07 -3.5075358E-06 7.8332869E-06 1.381244E-05 -1.38124E-05 -1.38124	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6666011E-03 -8.3326185E-04 -6.2100174E-05 4.8007844E-06 5.6435969E-07 -1.63524648E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 1.1075391E-04 -1.2986703E-05 -4.9693762E-05 -1.03531E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.3907837E-02 -1.42973564E-02 -1.22924910E-02 -6.7413567E-03 -2.5546250E-03 -1.4766257E-03 -3.8.0945657E-04 -4.0601852E-04 -1.700306E-04 -3.052716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.0252173E-02 -2.4170697E-03 -1.02529869E-02 -1.2529869E-02 -1.7532300E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.192755E-04 -2.1018983E-04 -8.8049493E-05 -1.5655586E-05 1.2056324E-07 -4.1038958E-08 -0.664724E-07 1.4162013E-07 -4.1038958E-08 -9.6061333E+00 -2.0416597E-05 7.1672253E-05 -2.053337E-04	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -6.1904548E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -3.7581084E-04 -2.0623615E-04 -2.063615E-04 -1.9317466E-07 -6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -3.6031104E-04 -2.651064E-04 -3.6051104E-04 -3.605104E-04 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.65506E-05 -5.56506E-	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486954E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -2.3230106E-04 -1.4537414E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 -2.632237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 192\\ 180\\ 180\\ 180\\ 180\\ 180\\ 180\\ 180\\ 180$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.61463658-02 6.7145353E-02 1.2474818E-01	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.2965670E-02 -3.2965670E-02 -7.3479864E-03 -1.2669461E-02 -7.3479864E-03 -2.0258641E-03 -8.4844613E-04 -1.5105779E-04 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -3.5075358E-02 -7.5278375E+02 9.0965057E-07 -3.5075358E-06 -1.3812446E-05 -1.81246E-05 -1.81	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0705194E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -8.6643540E-03 -5.2369602E-03 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 -4.8007844E-06 -1.6195221E-06 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 1.1075391E-04 -1.9489646E-04 -1.9489646E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-03 -2.554625E-03 -3.054557E-04 -3.052716E-02 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 4P- -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.504068E-04 -3.7507757E-04	1.5994258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.0475076E-02 -7.7832300E-03 -5.3347585E-03 -2.1893129E-03 -1.3236088E-03 -1.3236088E-03 -7.6449145E-04 -4.1927555E-04 -2.1018983E-04 -1.5655586E-05 -1.5655586E-05 -1.5655586E-05 -1.5655586E-05 -2.0645724E-06 -4.1038958E-08 -2.0416597E-05 -2.0416597E-05 -2.0535337E-04 -2.7390373E-04 -2.0553537E-04 -2.055537E-05 -2.0553537E-04 -2.055537E-05 -2.055537E-04 -2.055537E-04 -2.055337E-04 -2.0555582E-05 -2.055537E-04 -2.0555582E-05 -2.055537E-04 -2.055537E-04 -2.0555582E-05 -2.055537E-04 -2.055537E-04 -2.0555582E-05 -2.055537E-04 -2.055537E-04 -2.055537E-04 -2.055537E-04 -2.055537E-04 -2.055537E-04 -2.0555558E-05 -2.0555357E-05 -2.0555357E-05 -2.0555357E-05 -2.0555537E-04 -2.0555537E-04 -2.0555558E-05 -2.0555537E-04 -2.0555537E-04 -2.0555537E-04 -2.0555537E-04 -2.055555E-05 -2.05555557E-05 -2.055555	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7581084E-04 -2.6224758E-03 -7.6940850E-06 -7.6940850E-06 -7.6940850E-06 -7.6940880E-08 -2.0107018E-08 -2.0310064E-04 -5.6527686E-05 -6.1665581E-03 -3.0303104E-02 -0.40070E-05 -1.2849029E+00	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904465E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.6516478E-03 -1.1572758E-03 -7.589774E-04 -4.7486954E-04 -2.8728442E-04 -9.0988010E-05 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-05 -2.7850367E-05 -1.3957078E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 -7.9906891E-08 -2.6932237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 141\\ 141\\ 175\\ 176\\ 177\\ 180\\ 181\\ 141\\ 141\\ 141\\ 141\\ 141\\ 141\\ 141$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.5348452E+04 3.4144729E+04 7.7552073E+04 1.831766E+05 3.2312890E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.5367332E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -1.2669461E-02 -7.3479864E-03 -2.0258641E-03 -3.2464613E-04 -1.5105779E-04 1.1704689E-05 -3.94891441E-06 -3.9481149E-07 -3.9481149E-07 -3.9481149E-07 -3.5278375E+02 -1.3812446E-05 -1.381246E-05 -1.3812446E-05 -1.3812446E-05 -1.3812446E-05 -1.3812446E-05 -1.381246E-05 -1.3812446E-05 -1.381246E-05 -1	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7725194E-02 -4.7564793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 1.1075391E-04 -1.9489646E-04 3.0504688E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.147306E-02 -1.42973564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -2.554250E-03 -2.554250E-03 -2.554250E-04 -1.700306E-04 -3.052716E-05 2.3357655E-06 -7.8752411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 -1.0047874E-03	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.2529869E-02 -7.782300E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.192755E-04 -2.1018983E-04 -8.8049493E-05 -1.565586E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08 -9.6061333E+00 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 -2.7390373E-04 -4.9867871E-04	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -4.330889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.6516478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486554E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.4537414E-05 -2.7880367E-05 -3.848481E-06 -1.0393242E-06 -1.0393242E-06 -3.932237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182 \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823B+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -1.2669461E-03 -4.0327727E-03 -2.0288641E-03 -4.0327727E-03 -2.0288641E-03 -3.9489441E-06 -3.9489441E-06 -3.9489441E-06 -3.9881149E-07 -7.5278375E+02 9.0965057E-07 -3.5075358E-06 7.832869E-06 -1.8312446E-05 2.1716136E-05 -3.2222716E-05	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3326185E-04 -6.2100174E-05 -4.8007844E-06 -1.6195221E-06 5.643594E-07 -1.6854648E-07 -1.8645886E+02 -1.2896703E-05 -1.075391E-04 -1.9489646E-04 -1.9489646E-04 -1.488269E-07 -1.488269E-04 -1.488529E-04 -1.4	2.3275860E-02 5.0595306E-02 2.741076E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-03 -1.4766257E-03 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 1.459468E-03	1.5994258E-02 3.1409317E-02 1.6222173E-02 1.6222173E-02 1.025434E-02 1.2529869E-02 1.0475076E-02 7.7832300E-03 3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -1.3236088E-03 7.64449145E-04 -4.1927555E-04 -2.1018983E-04 -3.8049493E-05 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08 5P- -9.6061333E-00 -2.0416597E-05 -2.0535337E-04 2.7390373E-04 4.9867871E-04 2.6902937E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -7.6940850E-04 -2.0623615E-04 -1.9917466E-07 -6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527666E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -5.3380006E-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.2742441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.793253E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 -2.6332237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 178\\ 179\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 4.531828+04 3.4144729E+06 3.231280E+06 3.231280E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.058861E-01	6.0105809E-06 -1.4693522E-04 -3.31039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0527458E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -2.5278375E+02 9.0965057E-07 -3.5075358E-06 7.8332869E-06 -1.3812446E-05 2.1716136E-05 -3.24242716E-05 -3.242716E-05 -3.2427	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.30506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6155221E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -1.9693762E-05 1.1075391E-04 -1.9489646E-04 3.0504688E-04 -1.9489249E-04 -1.9489646E-04 3.0504688E-04 -1.9489249E-04 -1.9489249E-04 -1.9489249E-04 -1.9489249E-04 -1.9489249E-04 -1.949564E-04 -1.9489249E-04 -1.9489248E-04 -1.9489248E-04 -1.9489248E-04 -1.9489248E-04 -1.9489248E-04 -1.9489248E-04 -1.9489248E-04 -1.9489248E-04 -1.948948E-04 -1.94894	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.24766257E-03 -2.554260E-03 -2.554260E-03 -1.4766257E-04 -4.061852E-04 -1.700306E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 4P- -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 -1.4554968E-03	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -1.3236088E-03 -7.6444915E-04 -4.192755E-04 -4.192755E-04 -2.1018983E-03 -1.5655586E-05 -1.565538E-08 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 -2.730373E-04 -4.9867871E-04 2.9228815E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.77203202E-03 -1.7762097E-03 -5.1517130E-04 -3.7561084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.0107018E-08 -2.6310064E-04 -5.6527666E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -5.3380006E-01	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.6516478E-03 -1.1572758E-03 -1.5897747E-04 -4.7486954E-04 -2.782842E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.4537414E-05 -2.7850367E-05 -5.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.0393242E-09 -2.6932237E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.4102964E+06 2.9216892E+07 9.411732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.005861E-01 1.488731FE+00	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -2.0258641E-03 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -2.5278375E+02 9.0965057E-07 -3.5075358E-06 -1.3812446E-05 2.1716136E-05 -3.2242716E-05 4.6495084E-05 -4.6495084E-05	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -2.1009571E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3326185E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 -1.6195221E-06 -1.6354648E-07 -1.8645886E+02 -1.2896703E-05 -4.9693762E-05 1.1075391E-04 -1.9499646E-04 -1.9498646E-04 -1.9498646E-04 -1.9498646E-04 -1.9498646E-04 -1.949864E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -1.473564E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-03 -8.0945657E-04 -1.40601852E-04 -1.7000306E-04 -3.0252716E-05 2.3357655E-06 2.3357655E-06 7.78728211E-07 -7.8782411E-07 -7.8782411E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 4.0504068E-04 -1.0047874E-03 1.4554968E-03 -1.9025030E-03	1.5984258E-02 3.1409317E-02 1.6222173E-02 -2.4170697E-03 -1.1035434E-02 -1.2529869E-02 -1.2529869E-03 -5.3347585E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915-03 -7.6444915-03 -7.644915-03 -7.644915-03 -1.3655586E-05 -1.2555586E-05 -1.2565586E-05 -1.2565586E-05 -1.2056324E-06 -4.0646724E-07 -4.1038958E-08 -5P- -9.6061333E+00 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 2.7390373E-04 4.9867871E-04 2.6902937E-03 2.922815E-02 2.8313912F-01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -6.1904548E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04 -3.7581084E-04 -2.0623615E-04 -1.0333632E-04 -3.7581084E-04 -2.0623615E-06 -7.6940850E-06 -3.9107018E-08 -2.0107018E-08 -2.0107018E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -5.3380006E-01 -4.3202646E-01 1.3477392F-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.27322183E-03 -2.2742441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -1.6581658E-04 -1.6581658E-04 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-04 -3.5430106E-05 -5.0760481E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 3.4144729E+04 7.7552073E+04 4.531823E+05 1.1774969E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 9.7128202E+07 9.4711732E+08 1.3384720E+09 5.5667382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7164358E-02 1.2474818E-01 2.3178217E-01 8.0058661E-01 1.4887931E+00	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 -1.5105779E-04 -3.9489441E-06 1.3761821E-06 -3.9481449E-07 -2.5278375E+02 9.0965057E-07 -3.5975388E-06 -1.3812446E-05 -3.12446E-05 -3.242716E-05 -3.242716E-05 -4.6495084E-05 -6.4267822E-05 -6.4267822E-05 -5.4765054E-05 -6.4267822E-05 -5.4765054E-05 -5.4267822E-05 -5.4267826782 -5.4267826782 -5.4267827878788 -5.4678787878	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.3056359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -3.0292815E-03 -1.6606011E-03 -3.326185E-04 -3.4885394E-04 -6.2100174E-05 -4.8093762E-05 -1.6354648E-07 -1.86458866E-02 1.2896703E-05 -1.9693762E-05 1.1075391E-04 -1.9489646E-04 3.0504688E-04 -3.3616964E-04 -3.331287E-04 -3.	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.3907837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -4.2282845E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -2.357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 4P- -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 -1.9025030E-03 2.3062452E-03	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -1.3250682E-03 -7.6444915E-04 -4.192755E-04 -2.1013983E-04 -2.1013983E-04 -2.1013985E-08 -2.6661333E+00 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 -2.730373E-04 -4.9867871E-04 4.6902937E-03 -9.928415E-02 2.8313912E-01 -2.28415E-02 2.8313912E-01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.77203202E-03 -1.77203202E-03 -1.77203202E-03 -1.77203202E-03 -5.517133E-04 -2.622615E-04 -2.623613E-04 -4.3308889E-05 -7.6940850E-06 -7.6940850E-06 -2.6310064E-04 -5.527686E-05 -1.2849029E+00 -2.6310064E-04 -5.6327686E-05 -3.6031104E-02 -2.4163851E-01 -5.380006E-01 -4.320264E-01 1.3477329E-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -7.5897747E-04 -1.1572758E-03 -7.5897747E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.3957078E-05 -2.7850367E-05 -3.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.0393242E-09 -2.6932237E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 181\\ 182\\ 183\\ 184\\ 185\\ 163\\ 164\\ 165\\ 166\\ 167\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 162\\ 184\\ 185\\ 162\\ 162\\ 162\\ 162\\ 162\\ 162\\ 162\\ 162$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7761809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.831766E+05 4.531823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 2.5314129E+10 1.384720E+09 2.5314129E+10 1.9453737E=02 3.6141658E=02 6.7145353E+02 2.3178217E=01 4.3071120E=01 8.0058681E=01 4.3071120E=01 8.0058681E=01 4.3071120E=01 8.0058681E=01 4.3071120E=01 8.0058681E=01 4.3071120E=01 8.0058681E=01 4.3071120E=01 8.0058681E=01 4.3071120E=01 4.3071	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -8.4844613E-04 -1.5105779E-04 1.3761821E-06 -3.9881149E-07 -3.9881149E-07 -3.577535E+02 9.0965057E-07 -3.5075358E-06 7.832809E-06 -1.3812446E-05 2.1716136E-05 -3.242716E-05 4.6495084E-05 -6.4267822E-05 9.7062275E-05	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3326185E-04 -6.2100174E-05 4.8007844E-06 5.6435969E-07 -1.63524648E-07 -1.6354648E-07 -1.845886E+02 1.2896703E-05 -4.9693762E-05 1.1075391E-04 -1.9489646E-04 3.0504688E-04 -4.488289E-04 -4.488289E-04 -9.0331287E-04 1.336035E-03 -4.9633762E-05 -4.9693762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762E-05 -5.9695762	2.3275860E-02 5.0595306E-02 2.7410756E-02 -2.7410756E-02 -2.3907837E-02 -2.3907837E-02 -2.3907837E-02 -1.473564E-02 -1.0294910E-02 -6.7413567E-03 -2.5546250E-03 -1.4766257E-03 -3.0252716E-05 2.3357655E-0 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.6168113E+01 -4.6394948E-05 1.6870164E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 2.3062452E-03 -7.9202460E-03 2.3062452E-03	1.5984258E-02 3.1409317E-02 1.622173E-02 1.622173E-02 1.025434E-02 1.2529869E-02 1.2529869E-03 5.3347585699E-03 3.4955699E-03 1.3236088E-03 7.6444915E-04 4.1927555E-04 7.644915E-04 4.1927555E-04 7.644915E-04 4.1927555E-04 1.2056324E-06 1.2056324E-06 4.0646724E-07 1.4162013E-07 -4.1038958E-08 5P- -9.6061333E+00 -2.0416597E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 2.0535337E-04 4.9867871E-04 2.8313912E-01 6.8725142E-01 -2.0416297E-05 7.642937E-03 2.922815E-03	8.6821874E-03 1.6152076E-02 8.313029E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -5.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -3.7581084E-04 -2.0623615E-04 -4.330889E-05 -7.6940850E-06 5.9103384E-07 -1.917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527666E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -5.3380006E-01 -1.3477329E-01 4.8905387E-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -7.5897747E-04 -4.7486954E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -3.3949229E-06 2.608264E-07 -1.910714E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.4537414E-04 -2.7850367E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 -2.6392237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 9.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 1.2474818E-01 2.3178217E-01 1.2474818E-01 2.3178217E-01 1.2474818E-01 2.3178217E-01 1.2474818E-01 2.3178217E-01 1.2474818E-01 2.3178217E-01 1.2474818E-01 2.3178217E-01 1.2474818E-01 2.3178217E-01 2.3178217E-01 3.0058681E-01 1.4887931E+00 5.1625848E+00	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 -1.5105779E-04 -3.9881149E-07 -3.9881149E-07 -7.5278375E+02 9.0965057E-07 -3.5975358E-06 -1.3812446E-05 2.1716136E-05 -3.242716E-05 -3.242716E-05 -3.242716E-05 -3.242716E-05 -3.242716E-05 -3.242716E-05 -3.242716E-05 -1.2442494E-04 -1.242494E-04	2.2053270E-02 5.0989297E-02 5.0989297E-02 4.0725194E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -3.0375011E-02 -1.3787754E-02 -3.0375011E-02 -3.0292815E-03 -1.66606011E-03 -3.0292815E-03 -1.6606011E-03 -3.4885394E-04 -3.4885394E-04 -3.4885394E-04 -1.6195221E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 -1.9693762E-05 -1.9693762E-05 -4.9893762E-05 -1.94893646E-04 3.0504688E-04 -3.916964E-04 -3.916964E-04 -3.31287E-04 -1.33035E-03 -1.5944229E-03	2.3275860E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.147306E-02 -1.4973564E-02 -1.294910E-02 -6.7413567E-03 -4.2282845E-03 -4.2282845E-03 -2.554250E-03 -1.4766257E-03 -8.0945657E-04 -3.0525716E-05 -3.357675E-04 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 -1.9025030E-03 2.3062452E-03 -7.9029406E-03 -1.9025030E-03 2.3062452E-03 -7.9029406E-03 -1.1019740E-01	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529865E-03 -3.4955699E-03 -3.4955699E-03 -2.1893129E-03 -7.6444915E-04 -4.1927555E-04 -4.1927555E-04 -2.1018982E-04 -2.1018982E-04 -2.1018982E-04 -2.1018982E-04 -2.0416597E-05 7.1672253E-05 -2.653537E-04 2.7390373E-04 -2.0416597E-05 7.1672253E-05 2.1672253E-05 2.1672253E-05 2.1672253E-05 2.1672253E-05 2.1672253E-05 2.928815E-02 2.8313912E-01 3.1341941E-01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -5.151730E-04 -3.7581084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.0107018E-08 -2.6310064E-04 -5.6327686E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -3.36031104E-02 -2.4163851E-01 -3.36031104E-02 -2.4163851E-01 -3.36031104E-02 -2.4163851E-01 -3.36037E-01 -4.3905487E-01 2.1541172E-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -7.5897747E-04 -1.1572758E-03 -7.5897747E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 3.0630467E-08 -8.7921529E-08 3.0630467E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.7392532E-05 -5.0760481E-05 -2.7880367E-05 -1.3957078E-05 -1.3957078E-05 -1.3957078E-05 -2.6932237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.5348452E+04 7.7552073E+04 1.8331766E+05 3.2312890E+06 9.4102964E+06 2.9216992E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867332E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 1.4887931E+00 2.707233E+00 5.625848E+00 9.6361639E+00	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 -3.9489141E-06 -3.9489141E-06 -3.9481149E-07 -3.5278375E+02 9.0965057E-07 -3.5075358E-06 7.8332869E-06 -1.3812446E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.242242494E-04 1.4800346E-04	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6660611E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 5.6435969E-07 -1.63524648E-07 -1.6354648E-07 -1.8645886E+02 -1.9896703E-05 -1.9693762E-05 1.1075391E-04 -1.94896468E-04 -1.94896468E-04 -1.94896468E-04 -1.94896468E-04 -1.94896468E-04 -1.94896468E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.9489646E-04 -1.348028E-03 -1.5944229E-03 -1.5944229E-03 -1.5944229E-03	2.3275860E-02 5.0595306E-02 2.7410756E-02 -2.7410756E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -1.42973564E-02 -1.2294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-04 -2.5546250E-03 -1.4766257E-04 -3.052716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.6168113E+01 -4.65040608E-04 -3.7507757E-04 4.5040608E-03 -1.0047874E-03 1.4554968E-03 -1.9025030E-03 -3.3062452E-03 -7.9029460E-03 -1.1019740E-01 -5.4657109E-01	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.0252173E-02 -1.2529869E-02 -1.2529869E-03 -3.4955699E-03 -3.4955699E-03 -3.4955699E-03 -1.3236088E-03 -7.644915E-04 -4.192755E-04 -2.1018983E-04 -8.8049493E-05 -1.5655586E-05 -1.2056324E-06 -4.0646724E-07 -4.1038958E-08 -2.0416597E-05 7.167253E-05 -2.0535337E-04 -2.390373E-04 -4.9867871E-04 2.6902937E-03 2.9228815E-02 2.8313912E-01 6.8725142E-01 -3.141941E-01 -4.8407881E-01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -6.1904548E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -3.7581084E-04 -2.0623615E-04 -3.7581084E-04 -2.0638859E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -3.380006E-01 -3.3202646E-01 -3.3202646E-01 -3.3202646E-01 -3.3202646E-01 -3.3477329E-01 4.3905387E-01 -2.2646971E-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.27322183E-03 -2.2742441E-03 -1.6516478E-03 -7.5897747E-04 -4.7486954E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.792152E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -2.3230106E-04 -1.4537414E-04 -3.5430612E-04 -3.5430612E-04 -3.5430612E-05 -3.7480367E-05 -3.8484891E-06 -1.0393242E-06 7.9906891E-08 -2.632237E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.5348455E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 8.0058681E-01 1.4387312E+01 2.3178217E-01 8.0058681E-01 1.4387312E+01 2.3178217E-01 2.3178217E-01 2.3178217E-01 2.3178217E-01 2.3178217E-01 2.3178217E-01 2.361635E+00 5.1625848E+00 9.6361639E+00	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -6.9734773E-02 -3.2965670E-02 -3.2965670E-02 -7.3479864E-03 -4.0527727E-03 -2.025864E-03 -4.0327727E-03 -2.025864E-03 -2.025864E-03 -2.025864E-03 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -7.5278375E+02 9.0965057E-07 -3.5975358E-06 -1.3812446E-05 2.1716136E-05 -3.2242716E-05 -3.2242716E-05 -3.2242716E-05 -3.2242716E-05 -3.2242716E-05 -3.2242716E-05 -1.2442494E-04 1.4800346E-04 .3.436015E-04	2.2053270E-02 5.0989297E-02 5.0989297E-02 4.0725194E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -5.2369602E-03 -1.6606011E-03 -8.3226185E-04 -3.4885394E-04 -6.2100174E-05 -6.435969E-07 -1.6354648E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 -4.9693762E-05 -4.9693762E-05 -4.9693762E-05 -4.9693762E-05 -4.9693762E-05 -4.9693762E-05 -4.9693762E-05 -4.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9893762E-05 -5.9993762E-05 -5.9	2.3275860E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -2.147306E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -4.2282845E-03 -2.554250E-03 -1.4766257E-03 -2.554250E-03 -2.554250E-03 -3.40567E-04 -3.052716E-05 -3.357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 -1.9025030E-03 2.3062452E-03 -7.9029406E-03 -1.1019740E-01 -5.433775FE-01	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.529869E-02 -1.2529869E-02 -1.32529865E-03 -3.4955699E-03 -2.1893129E-03 -7.6444915E-04 -4.1927555E-04 -1.3250682E-03 -1.3250682E-03 -1.5655586E-05 -1.5655586E-05 -1.5655586E-05 -1.5655586E-05 -2.0535337E-04 -2.0416597E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 7.1672253E-05 2.0535337E-04 -2.0416597E-05 7.1672253E-05 2.0535337E-04 -2.0416597E-05 7.1672253E-05 2.053537E-04 2.9228815E-02 2.8313912E-01 3.1341941E-01 -4.54807881E-01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -6.5117130E-04 -2.6224758E-03 -1.033633E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6327666E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -3.3603104E-02 -2.4163851E-01 -4.3202646E-01 1.3477329E-01 -2.1541172E-01 -2.2646971E-01 -2.2646971E-01 -2.21160347E-01	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.398415E-03 -2.7322183E-03 -2.7322183E-03 -7.5897747E-04 -1.1572758E-03 -7.5897747E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 3.0630467E-08 -8.7921529E-08 3.0630467E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.357078E-05 -2.7650367E-05 -2.7850367E-05 -1.3957078E-05 -1.3957078E-05 -3.5484891E-06 -1.0393242E-06 2.906891E-08 -2.90821E-08 -2.932237E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 180\\ 187\\ 188\\ 180\\ 180$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.5348452E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 3.2312890E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.410294E+06 9.410294E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867332E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 6.7145353E-02 6.7145353E-01 1.247481E-01 2.3178217E-01 4.3071120E-01 1.4887931E+00 2.7707233E+00 5.162584E+00 9.6361639E+00 1.8031447E+01 1.38847E-01	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -1.2669461E-02 -7.3479864E-03 -2.0258641E-03 -2.0258641E-03 -3.94894418E-06 -3.948944182-06 -3.948144613E-04 -1.5105779E-04 -3.94814413E-06 -3.94814413E-07 -3.9483149E-07 -3.9483149E-07 -3.9483149E-07 -3.5275355E+02 -1.3812446E-05 -1.3812446E-05 -1.3812446E-05 -1.3812446E-05 -1.342442E-05 9.7062275E-05 -1.2442494E-04 1.4800346E-04 -3.4346015E-04 -3.4346015E-04 -3.4346015E-04	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.7154793E-02 -4.7564793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07 -1.6354648E-07 -1.8645886E+02 -1.2896703E-05 -1.948964E-04 3.0504688E-04 -3.488529E-04 -1.948964E-04 3.0504688E-04 -4.488298E-04 -1.948964E-04 -3.0504688E-04 -4.488298E-04 -1.948964E-04 -3.0504688E-04 -4.488298E-04 -1.948964E-04 -3.0504688E-04 -4.381529E-03 3.8354015E-03 -1.5944229E-03 3.8354015E-03 -3.202907E-04	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.3907837E-02 -1.42973564E-02 -1.2294910E-02 -6.7413567E-03 -4.2282845E-03 -1.4766257E-03 -2.554250E-03 -2.554250E-03 -2.354765E-04 -3.052716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.6168113E+01 -4.6168113E+01 -4.504060E-04 -3.7507757E-04 -1.0047874E-03 1.4554968E-03 2.3062452E-03 -7.9029460E-03 2.3062452E-03 -7.9029460E-01 -5.4657109E-01 -5.4657109E-01	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.0252478E-02 -2.4170697E-03 -1.02524869E-02 -1.2529869E-02 -1.2529869E-03 -3.4955699E-03 -2.1893129E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.644915E-04 -4.192755E-04 -2.1018983E-04 -8.8049493E-05 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 -2.7390373E-04 -4.9867871E-04 2.922837E=03 -2.92387E=03 -2.92387E=03 -2.92387E=03 -3.1341941E=01 -4.8407881E=01 -4.849382E-01 -4.2481993E=01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.7581084E-04 -2.6224758E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -3.7581084E-07 -4.330889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -3.380006E-01 -3.380064E-04 -5.3527686E-05 -6.1665581E-01 -3.380006E-01 -3.380064E-04 -5.380064E-04 -2.4163851E-01 -2.2468971E-01 -2.2646971E-01 -2.160347E-01 -1.580304E-07 -2.160347E-01 -2.160347E-01 -2.160347E-01 -1.580304E-07 -2.160347E-01 -2.160347E-01 -2.160347E-01 -2.160347E-01	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -2.7422441E-03 -1.6516478E-03 -7.5897747E-04 -4.7486554E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.3557078E-05 -3.7480367E-05 -3.8484891E-06 -1.0393242E-06 -1.0393242E-06 -3.0392787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E+00 2.7707233E+00 9.6361639E+00 1.8331447E+01 3.858337E+01 3.858337E+01 3.858337E+01 3.858337E+01 3.858337E+01	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.2965670E-02 -3.2965670E-02 -7.3479864E-03 -1.2669461E-02 -7.3479864E-03 -1.2669461E-02 -7.3479864E-03 -2.0258641E-03 -8.4844613E-04 -1.5105779E-04 1.1704689E-05 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -7.5278375E+02 9.0965057E-07 -3.5075358E-06 -7.8322869E-06 -1.3812446E-05 2.1716136E-05 -3.242716E-05 -4.6495084E-05 -5.242716E-05 -4.6495084E-05 -1.242494E-04 1.4800346E-04 -3.434615E-04 4.9628044E-04 -3.434615E-04 4.9628044E-04 -3.434615E-04	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.0397754E-02 -8.6643540E-03 -5.2369602E-03 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3326185E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 -5.6435969E-07 -1.6354648E-04 -1.2896703E-05 -4.9693762E-05 1.1075391E-04 -1.948964E-04 -4.488289E-04 -4.3916964E-04 -4.488289E-04 -3.305468E-04 -4.488289E-04 -3.31287E-04 -1.948964E-04 -1.948964E-04 -1.948964E-04 -3.3654648E-04 -4.488289E-04 -3.3654648E-04 -4.488289E-04 -3.3654648E-04 -3.3654648E-04 -3.3654648E-04 -3.3654648E-04 -3.4633546E-03 -4.5783363E-02 3.8354015E-03 -4.5783363E-02 3.2042697E-01 -5.7644229E-03 -5.76345229E-03 -5.7644229E-03 -5.774424284584848484848484848484848484848484	2.3275860E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -2.147306E-02 -1.4973564E-03 -4.228249410E-02 -6.7413567E-03 -1.4766257E-03 -2.554625E-03 -3.0945657E-04 -3.052716E-04 -3.052716E-02 -3.357655E-06 -7.8782411E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 -1.49254068E-03 -1.49254068E-03 -1.49254068E-03 -1.49254068E-03 -1.49254068E-03 -1.49254068E-03 -1.49254068E-03 -1.4554968E-03	1.5994258E-02 3.1409317E-02 1.6222173E-02 1.6222173E-02 1.025434E-02 1.2529869E-02 1.2529869E-03 5.3347585E-03 3.4955699E-03 1.3236088E-03 1.3236088E-03 1.3236088E-03 1.3236088E-03 1.41927555E-04 -2.1018933E-04 4.1927555E-04 -2.1018933E-04 4.0646724E-07 1.4162013E-07 -4.1038958E-08 5P- 9.6061333E+00 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 2.7390373E-04 4.9867871E-04 2.6902937E-03 2.922815E-02 2.8313912E-01 6.8725142E-01 3.1341941E-01 -4.5481993E-01 4.5491993E-01 4.5491993E-01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -5.51103E-04 -3.7581084E-04 -2.0623615E-04 -3.7581084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 -7.6940850E-06 -7.6940850E-06 -7.6940850E-06 -7.6940850E-06 -7.6940850E-06 -7.6940850E-06 -7.6940850E-06 -7.6940850E-08 -2.0107018E-08 -2.0310064E-04 -5.358006E-01 -3.36031104E-02 -2.4163851E-01 1.3477329E-01 1.4.8905387E-01 -2.160347E-01 1.541172E-01 1.5892391E-02 -2.160347E-01 1.5892391E-02	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 -2.27322183E-03 -2.27322183E-03 -2.2742441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.793253E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 -1.0393242E-06 -7.9906891E-08 -2.6932237E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 178\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 3.5348452E+04 3.4144729E+04 7.7552073E+04 4.531823E+05 3.4141728E+06 3.2312890E+06 3.2312890E+06 3.431280E+06 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.058681E-01 1.4887931E+00 5.162548E+00 2.5162548E+00 9.6361639E+00 1.8031447E+01 3.38837E+01 6.3875692E+01	6.0105809E-06 -1.4693522E-04 -3.31039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.025864E-03 -2.025864E-03 -2.025864E-03 -2.025864E-03 -3.9489441E-06 1.3761821E-06 -3.9489141E-07 -2.5278375E+02 -7.5278375E+02 -1.3812446E-05 -1.3812446E-05 -1.3812446E-05 -1.382424E-04 -1.382424E-05 -1.242424E-04 -1.242424E-04 -1.242424E-04 -1.24460584E-04 -3.2486084E-04 -1.242424E-04 1.2446044E-04 -1.242424E-04 1.244242E-04 1.244242E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.24242E-04 1.242424E-04 1.24242E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.242424E-04 1.24242E-04 1.242424E-04 1.24242E-04 1.242424E-04 1.24242E-04 1.24242E-04 1.242424E-04 1.24242E-04 1.24242E-04 1.24242E-04 1.242424E-04 1.24242E-04 1.242424E-04 1.24242E-04 1.24242E-04 1.242424E-04 1.24242E-04 1.2422E-04 1.242E	2.2053270E-02 5.0989297E-02 5.0989297E-02 4.0725194E-02 4.7154793E-02 4.7154793E-02 4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6155221E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 1.1075391E-04 3.0504688E-04 -1.9489646E-04 3.0504688E-04 -1.9489646E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.34635E-03 3.8354015E-03 3.2042697E-01 5.3506410E-01	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -4.2282845E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -2.554250E-04 -1.7000306E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4P- -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 2.3062452E-03 -7.9029460E-03 2.3062452E-03 -7.9029460E-03 1.019740E-01 -5.4657109E-01 -5.4657109E-01 4.6050660E-01	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -1.3236698E-03 -3.4955699E-03 -2.1893129E-03 -3.4955699E-03 -1.3236088E-03 -7.6444915E-04 -4.192755E-04 -4.192755E-04 -2.1018983E-04 -2.1018983E-05 -1.565556E-05 -1.565556E-05 -1.565556E-05 -1.665558E-05 -1.665558E-08 -2.053537E-04 2.7390373E-04 -2.902416597E-05 7.1672252E-05 7.1672252E-05 7.1672252E-05 -2.053537E-04 2.7390373E-04 -2.92881E-02 2.8313912E-01 6.8725142E-01 -4.48407881E-01 -4.5481993E-01 -4.2390518E-02 2.4979948E-01	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.7762097E-03 -2.6224758E-03 -1.7203202E-03 -1.7762097E-03 -6.5117130E-04 -2.6623615E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527668E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -5.3380006E-01 1.3477329E-01 4.3905387E-01 -2.2646971E-01 -2.2646971E-01 -2.2646971E-01 1.5892391E-02 1.0529281E-01	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.6516478E-03 -7.5897747E-04 -4.7486954E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.4537414E-05 -2.7850367E-05 -5.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.0393242E-09 -2.6932237E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 167\\ 168\\ 169\\ 170\\ 171\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 188\\ 189\\ 190\\ 191\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823B+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 2.3178217E-01 4.3071120E-01 8.0058681E-01 2.3178217E-01 1.4887931E+00 2.7707233E+00 5.6361639E+00 1.8388337E+01 3.858337E+01 1.3858337E+01 1.3858337E+01 1.3858337E+01 1.8388337E+01 1.8388337E+01 1.8388337E+01 1.8388337E+01 1.8388337E+01 1.8388337E+01 1.8388337E+01 1.2125177E+02	6.0105809E-06 -1.4693522E-04 5.3310398E-03 -3.3138881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.9265670E-02 -3.9265670E-02 -2.0881919E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -8.4844613E-04 -1.5105779E-04 1.1704689E-05 -3.9489441E-06 1.3761821E-06 -3.9881149E-07 -3.988149E-07 -3.9065057E-07 -3.5275355E-06 -1.3312446E-05 -3.1242716E-05 -3.242716E-05 -4.495084E-03 -3.242716E-05 -4.495084E-04 1.4800346E-04 -3.4346015E-04 4.9628044E-04 1.40034612E-04 1.4800346E-04 -3.4346015E-04 4.9628044E-04 1.0051412E-02 1.0530040E-01	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0725194E-02 -4.0506359E-02 -3.0375011E-02 -1.378778E-02 -8.6643540E-03 -5.2369602E-03 -1.6606011E-03 -8.3326185E-04 -6.2100174E-05 4.8007844E-06 -1.6195221E-06 -1.6195221E-06 -1.6354648E-07 -1.8645886E+02 -1.8645886E+02 -1.2896703E-05 -4.9693762E-05 1.1075391E-04 -1.9499646E-04 -1.9499646E-04 -1.9499646E-04 -1.9499646E-04 -1.9499646E-04 -1.9499646E-04 -1.33165E-03 -3.5364415E-03 -3.5364415E-03 -3.5364415E-03 -3.53506410E-01 5.3506410E-01 2.2896636E-01	2.3275860E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -2.147306E-02 -1.4973564E-02 -1.2924910E-02 -6.7413567E-03 -2.554250E-03 -1.7000306E-04 -1.7000306E-04 -1.7000306E-04 -3.052716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 1.4554968E-03 -1.9025030E-03 2.3062452E-03 -7.9029460E-04 -1.019740E-01 -5.4357197E-01 -5.6337875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-01 1.3351790E-01 -5.6357875E-0	1.5994258E-02 3.1409317E-02 1.6222173E-02 1.0252173E-02 1.02529869E-03 1.1035434E-02 1.2529869E-03 5.3347585E-03 3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -2.1893129E-03 -1.3236088E-03 -1.3236088E-05 1.2056324E-06 4.1927555E-04 -2.1018983E-04 -2.1018983E-04 -3.8049493E-05 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 1.4162013E-07 -4.1038958E-08 -5.0661333E+00 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 2.7390373E-04 4.9867871E-04 2.8313912E-01 3.1341941E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407881E-01 -4.8407841E-01	8.6821874E-03 1.6152076E-02 8.313029E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -6.1904548E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -3.7581084E-04 -2.0623615E-04 -1.0333633E-04 -4.330889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 -6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -3.6031104E-04 -2.4163851E-01 -5.3380006E-01 -4.320264E-01 1.3477329E-01 4.8905387E-01 2.2646971E-01 -2.2160347E-01 1.5892391E-02 1.0529281E-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.27322183E-03 -2.2742441E-03 -1.15772758E-03 -7.5897747E-04 -4.7486954E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -8.7932532E-05 -2.7850367E-05 -1.3957078E-05 -5.8484891E-06 -1.0393242E-06 7.9906891E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.5348455E+04 3.4144729E+04 7.7552073E+04 4.831766E+05 4.531823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6414658E-02 6.7145358-02 1.2474818E-01 2.377120E-01 8.058661E-01 1.4887931E+00 2.7707233E+00 5.1625848E+00 9.6361639E+00 1.8031447E+01 3.3858337E+01 6.3875692E+01 1.2125177E+02 2.3200920E+02	6.0105809E-06 -1.4693522E-04 -5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.028641E-03 -2.028641E-03 -2.028641E-03 -3.9489441E-06 1.3761821E-06 -3.9489441E-06 1.3761821E-06 -3.9489441E-07 -2.5278375E+02 9.0965057E-07 -3.5975388E-06 -1.3812446E-05 2.1716136E-05 3.242716E-05 4.6495084E-04 -1.242494E-04 1.2467822E-05 9.7062275E-05 -1.2424294E-04 1.4800346E-04 -3.4346015E-04 4.9528044E-04 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01 1.0530040E-01	2.2053270E-02 5.0989297E-02 5.0989297E-02 4.0754794E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6360611E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.63554648E-07 -1.6354648E-07 -1.6354648E-07 -1.86458866E+02 -1.9489646E-04 3.0504688E-04 -1.9489646E-04 3.0504688E-04 -1.9489646E-04 3.0504688E-04 -1.9489646E-04 3.504688E-04 -1.36054E-04 -1.9489646E-04 3.504688E-04 -1.5944229E-03 3.8354015E-03 -1.5944229E-03 3.8354015E-03 -1.5944229E-01 5.3506410E-01 -2.2896636E-01 -1.0764924E-01	2.3275860E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -1.42973564E-02 -1.2294910E-02 -6.7413567E-03 -4.2282845E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -2.554250E-03 -3.0356755E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -1.0047874E-03 1.4554968E-03 -1.9025030E-03 2.3062452E-03 -7.9029460E-03 -1.9025030E-04 -1.0027874E-05 1.637875E-01 -5.6337875E-01 1.3351790E-01 4.6050660E-01 1.9198472E-01 -4.3998472E-01	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.2529869E-02 -1.2529869E-02 -1.32529868E-03 -3.4955699E-03 -2.1893129E-03 -3.4955699E-03 -1.323068E-03 -7.6444915E-04 -4.192755E-04 -4.192755E-04 -2.1018983E-04 -2.1018983E-05 -1.565586E-05 -1.565586E-05 -1.565532E-07 -4.1038958E-08 -2.0416597E-05 7.1672252E-05 -2.053337E-04 2.7390373E-04 -2.928815E-02 2.8313912E-01 6.8725142E-01 3.1341941E-01 -4.5481933E-02 2.4979948E-01 1.030065E-01 -2.089177E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -2.6224768E-03 -1.7203202E-03 -1.7762097E-03 -2.6224768E-03 -5.151308-04 -3.7581084E-04 -2.0623615E-04 -4.3308839E-05 -7.6940850E-06 -7.6940850E-06 -3.910384E-07 -6.9388206E-08 -2.0107018E-08 -2.0107018E-08 -2.0107018E-08 -2.6310064E-04 -5.6327666E-05 -6.1665581E-03 -3.6031104E-02 -2.463851E-01 -3.36005E-01 -4.3202646E-01 1.3477329E-01 2.1541172E-01 -2.2646971E-01 1.5892391E-02 1.0529281E-01 1.5892391E-02 1.0529281E-01 -8.4760406E-03	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.1572758E-03 -1.1572758E-03 -1.572758E-03 -2.872842E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.4537414E-05 -2.7850367E-05 -3.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.0393242E-09 -2.6932237E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7761809E+02 1.7450942E+03 3.534845E+03 7.3220404E+03 1.5571453E+04 7.7552073E+04 1.8331766E+05 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 6.7145353E-02 1.2474818E-01 2.3378217E-01 8.0058681E-01 1.4887931E+00 2.51625848E+00 9.6361639E+00 1.8031447E+01 3.3858337E+01 6.3875692E+01 1.2125177E+02 2.3200920E+02 4.4864177E+00	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 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$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 9.7128202E+07 9.7128202E+07 9.4711732E+08 1.3384720E+09 5.5667382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 1.2474818E-01 2.3178217E-01 2.3178217E-01 2.3178217E-01 2.3178217E-01 1.4387931E+00 5.1625848E+00 9.6361639E+00 1.8031447E+01 3.3858337E+01 6.3875692E+01 1.212517E+02 2.3200920E+02 4.4845175E+02 2.3200920E+02 4.776172E+02 2.3200920E+02	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 -1.5105779E-04 -3.9881149E-07 -3.9881149E-07 -3.9881149E-07 -3.9881149E-07 -3.9881149E-07 -3.9881149E-07 -3.9881149E-07 -3.292716E-05 -3.242716E-05 -3.242716E-05 -1.2442494E-04 1.3436015E-04 -3.436015E-04 -3.436015E-04 -3.436015E-04 -3.436015E-04 -3.436015E-04 -3.436015E-04 -3.2227155E-01 -1.2207155E-01 -3.237929E-01 -3.237929E-01	2.2053270E-02 5.0989297E-02 5.0989297E-02 4.0725194E-02 -1.1199777E-02 -4.7154793E-02 -4.7154793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6606011E-03 -8.3206185E-04 -3.4885394E-04 -6.2100174E-05 -4.3007844E-06 -1.6195221E-06 5.6435969E-07 -1.6354648E-07 -1.8645886E+02 1.2896703E-05 -4.9693762E-05 -4.9693762E-05 -1.9693762E-05 -1.9693762E-05 -4.9693762E-05 -1.9693762E-05 -1.931287E-04 -1.9489646E-04 3.0504688E-04 -1.9489846E-04 3.0504688E-04 -1.9489846E-04 3.0504688E-04 -1.948954E-04 -1.9489646E-04 3.0504688E-04 -1.948954E-04 -1.9489646E-04 3.20504688E-04 -1.33063402E-03 -1.5944229E-03 3.8354015E-03 3.2042697E-01 5.3506410E-01 -1.5944229E-03 3.2042697E-01 5.3506410E-01 -1.3662447E-01 -1.3642447E-01 -1.3629447E-01 -1.364747E-01	2.3275860E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -2.147306E-02 -1.0294910E-02 -6.7413567E-03 -4.2282845E-03 -4.2282845E-03 -2.554250E-03 -1.4766257E-03 -2.554250E-03 -2.554250E-03 -2.3547655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.3994948E-05 1.6870164E-04 -3.7507757E-04 6.5040608E-04 -1.0047874E-03 2.362452E-03 -1.9025030E-03 2.3062452E-03 -7.9029406E-03 -1.1019740E-01 -5.6337875E-01 1.351790E-01 4.650660E-01 -1.0457472E-01 -5.6337875E-02 -9.9267957E-02 -9.9267957E-02 -9.9267957E-02 -9.9267957E-02 -7.0874807E-02	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.529869E-02 -1.2529869E-02 -1.32529862E-03 -3.4955699E-03 -2.1893129E-03 -3.4955699E-03 -2.1893129E-03 -7.6444915E-04 -4.1927555E-04 -2.1013983E-04 -2.1013983E-04 -2.1013983E-04 -2.1013985E-03 -1.5655586E-05 -1.5655586E-05 -1.665533E+00 -2.063537E-04 -2.03937E-04 -2.03937E-04 -2.03937E-04 -2.03937E-04 -2.928815E-02 2.8313912E-01 3.1341941E-01 -4.5481993E-01 2.390518E-02 2.439948E-01 -2.0689177E-02 -4.7649979E-02 -4.764977E-02	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -5.1518739E-03 -3.8340378E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7203202E-03 -1.7581084E-04 -2.0623615E-04 -3.7581084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 -3.940850E-06 -3.940850E-06 -2.6310064E-04 -5.532606E-01 -3.36031104E-02 -2.4163851E-01 -3.36031104E-02 -2.4163851E-01 1.5323006E-01 1.3477329E-01 1.582331E-02 1.552281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.5528281E-02 1.	3.8867421E-03 7.2202503E-03 5.2904485E-04 -2.398415E-03 -2.7322183E-03 -2.7322183E-03 -7.5897747E-04 -1.1572758E-03 -7.5897747E-04 -2.872842E-04 -1.6581658E-04 -9.0988010E-05 -1.9107141E-05 -3.3949229E-06 3.0630467E-08 -8.7921529E-08 3.0630467E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -6.9638073E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.357078-05 -2.7850367E-05 -1.3957078-05 -1.3957078-05 -1.3957078-05 -3.5484891E-06 -1.0393242E-06 -1.0393242E-06 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 178\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 105\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.53484528+04 3.4144729E+04 7.7552073E+04 1.831766E+05 3.2312890E+06 3.2312890E+06 3.431232E+07 9.410294E+06 2.9216892E+07 9.410294E+06 2.9216892E+07 9.410294E+06 2.9216892E+07 9.410294E+06 2.9216892E+07 9.410294E+06 2.9216892E+07 3.471172E+08 1.384720E+09 2.5314129E+10 2.5314129E+10 2.53737E-02 3.6141658E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 5.1625848E+00 9.6361639E+00 1.8031447E+01 6.3875692E+01 1.2125177E+02 8.3356837E+01 6.3875692E+01 1.2125177E+02 8.7761809E+02 4.4845175E+02 8.7761809E+02	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -9.4791276E-02 -3.2965670E-02 -2.0881919E-02 -7.3479864E-03 -4.0327727E-03 -2.0258641E-03 -2.0258641E-03 -2.0258641E-03 -3.9489441E-06 1.3761821E-06 -3.94891441E-06 -3.94891441E-07 -7.5278375E+02 -7.5278375E+02 -7.5278375E+02 -1.381246E-05 -3.9489441E-06 -3.39881149E-07 -3.965057E-07 -3.5075358E-06 7.8332869E-06 -1.381244E-05 2.1716136E-05 -3.2422716E-05 -1.242424E-04 1.34601346E-04 -3.4346015E-04 4.9628044E-04 -3.4346015E-04 4.9628044E-04 -3.4346015E-04 2.7676550E-01 3.207155E-01 2.379262E-01 1.3379262E-01 1.3379262E-01 2.379262E-01 2.379262E-01	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.775194E-02 -4.7564793E-02 -4.0506359E-02 -3.0375011E-02 -1.3787754E-02 -8.6643540E-03 -5.2369602E-03 -3.0292815E-03 -1.6660011E-03 -8.3326185E-04 -3.4885394E-04 -6.2100174E-05 4.8007844E-06 -1.6155221E-06 5.6435969E-07 -1.6354648E-07 -1.6354648E-07 -1.8645886E+02 -1.9489646E-04 3.0504688E-04 -1.9489646E-04 3.0504688E-04 -1.9489646E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.948964E-04 3.0504688E-04 -1.594429E-03 3.8354015E-03 4.5783363E-02 3.2042697E-01 5.3506410E-01 2.2896636E-01 -1.3629447E-01 -1.3629447E-01 -1.3629447E-01 -1.3629447E-01 -7.3652942F-01	2.3275860E-02 5.0595306E-02 2.7410756E-02 -4.7571173E-03 -2.1062736E-02 -2.3907837E-02 -2.3907837E-02 -2.3907837E-02 -1.42973564E-02 -1.2294910E-02 -6.7413567E-03 -4.2282845E-03 -1.24766257E-03 -2.554250E-03 -2.554250E-03 -2.554250E-04 -1.700306E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4 -4.6168113E+01 -4.6168113E+01 -4.6504508E-04 -1.00047874E-03 1.4554968E-03 2.3062452E-03 -7.9029460E-03 1.4554968E-03 1.1019740E-01 -5.4657109E-01 -5.4657109E-01 -3.351709E-01 4.650660E-01 1.3351709E-01 4.650660E-01 1.9198472E-01 -5.4657109E-01 -4.5965987E-02 -9.9267957E-02 -7.0874802E-02	1.5984258E-02 3.1409317E-02 1.622173E-02 -2.4170697E-03 -1.035434E-02 -1.522866E-02 -1.2529865E-03 -3.4955699E-03 -2.1893129E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.192755E-04 -2.1018983E-04 -8.8049493E-05 -1.5655586E-05 1.2056324E-06 -4.0646724E-07 -4.1038958E-08 -2.0416597E-05 7.1672253E-04 -2.0416597E-05 7.1672253E-05 -2.0535337E-04 2.7390373E-04 -2.90237E-03 -2.083537E-04 2.9228415E-02 2.8313912E-01 6.8725142E-01 -4.8407881E-01 -4.28407881E-01 -4.28407881E-01 -4.28407881E-01 -4.28407881E-01 -4.28407881E-01 -4.28407881E-01 -4.28407881E-01 -2.068177E-02 2.497948E-01 1.0300065E-01 -2.068177E-02 -4.7649979E-02 -4.7649979E-02 -4.7649979E-02 -4.764997E-02 -4.764997E-02 -4.8405843E-02 -4.846843E-02 -4.8405843E-02 -4.846848E-02 -4.846848E-02 -4.846848E-02 -4.846848E-02 -4.846848E-02 -4.846848E-02 -4.	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -6.1904548E-03 -3.8340378E-03 -1.7203202E-03 -1.7203202E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -3.7581084E-07 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -6.6527686E-05 -6.1665581E-01 -3.6031104E-02 -2.4163851E-01 -5.338006E-01 1.3477329E-01 4.3905387E-01 1.5892391E-02 1.0529281E-01 1.5892391E-02 1.0529281E-01 4.36046E-03 -1.960406E-03 -1.9600133E-02 -1.4060746E-02	3.8967421E-03 7.2202503E-03 5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -2.7322183E-03 -1.6516478E-03 -1.1572758E-03 -7.5897747E-04 -4.7486554E-04 -2.8728442E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.6088264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -3.5430612E-04 -2.3230106E-04 -1.4537414E-04 -2.3230106E-04 -1.4537414E-05 -2.7850367E-05 -5.8484891E-06 -1.0393242E-06 -1.0393242E-06 -1.0393242E-08 9.3829787E-09 -2.7189798E-09
$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 167\\ 168\\ 167\\ 177\\ 178\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 186\\ 186\\ 187\\ 188\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823E+05 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 2.5314129E+10 2.5314129E+10 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4857337E+02 2.3778217E-01 1.4857337E+02 2.707233E+00 5.6361639E+00 1.8385337E+01 3.858337E+01 1.2125177E+02 2.3200920E+02 1.2125177E+02 2.3778109E+02 1.2125177E+02 2.3781809E+02 1.2125177E+02 2.3781809E+02 1.7450942E+03 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$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 3.5348455E+04 3.4144729E+04 7.7552073E+04 4.531823E+05 3.4144729E+06 3.2312890E+06 3.2312890E+06 3.2312890E+06 3.4714732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 3.4714732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 3.471473537E-02 3.641658E-02 1.2474818E-01 2.377120E-01 8.058681E-01 4.3071120E-01 8.058681E-01 1.4887931E+00 2.7707233E+00 5.162584E+00 3.3831447E+01 3.38837E+01 6.3875692E+01 1.2125177E+02 8.7781809E+02 1.745092E+03 3.5348455E+03	6.0105809E-06 -1.4693522E-04 -3.31039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -8.8657364E-02 -9.4791276E-02 -3.2965670E-02 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$\begin{array}{c} 150\\ 151\\ 152\\ 153\\ 154\\ 155\\ 156\\ 157\\ 158\\ 159\\ 160\\ 161\\ 162\\ 163\\ 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ \end{array}$	1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04 3.4144729E+04 7.7552073E+04 1.8331766E+05 4.5318823B+05 1.1774969E+06 3.2312890E+06 9.4102964E+06 2.9216892E+07 9.7128202E+07 3.4711732E+08 1.3384720E+09 5.5867382E+09 2.5314129E+10 1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.063681E-01 1.4887931E+00 5.6387639E+00 1.8031447E+01 3.3888337E+01 6.3875692E+01 1.2125177E+02 2.3200920E+02 4.4845176E+02 8.7781809E+02 1.7450942E+03 3.538485E+03 7.3220404E+03	6.0105809E-06 -1.4693522E-04 5.331039E-03 -3.313881E-02 -7.4346622E-02 -9.4791276E-02 -9.4791276E-02 -9.4791276E-02 -3.2965670E-02 -3.2965670E-02 -3.2965670E-02 -1.2669461E-02 -7.3479864E-03 -4.0327727E-03 -8.4844613E-04 -1.5105779E-04 -3.9489441E-06 -3.9489441E-06 -3.9489441E-06 -3.9489441E-07 -3.5075358E-06 7.832269E-06 -1.3612246E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -3.2422716E-05 -1.2442494E-04 -1.480346E-04 -3.4346015E-04 4.495084E-05 -1.2442494E-04 1.4800346E-04 -3.4346015E-04 1.480344E-04 1.480344E-04 1.480344E-04 1.480344E-04 1.480344E-04 1.480344E-04 1.480344E-04 1.480344E-04 1.480344E-04 1.3207155E-01 2.3379262E-01 1.3377488E-01 2.3379262E-01 1.3377488E-02	2.2053270E-02 5.0989297E-02 3.4317940E-02 -1.1199777E-02 -4.0706139E-02 -4.0506359E-02 -3.0375011E-02 -1.0377754E-02 -8.6643540E-03 -5.2369602E-03 -1.666011E-03 -8.3326185E-04 -1.6195221E-06 5.643594E-07 -1.63524648E-07 -1.63524648E-07 -1.6354648E-07 -1.6354648E-07 -1.845886E+02 1.2896703E-05 -4.9693762E-05 1.1075391E-04 -4.9693762E-05 1.1075391E-04 -4.9693762E-05 1.1075391E-04 -4.9693762E-05 1.1075391E-04 -3.8354015E-03 -4.5783363E-02 3.8354015E-03 -1.5944229E-03 3.8354015E-03 -1.5944229E-03 3.8354015E-03 -1.5944229E-03 3.8354015E-03 -1.5944229E-03 3.8354016E-04 -1.362944E-01 -1.362947E-01 -1.362947E-01 -1.362947E-01 -1.364107E-01 -7.395268E-02 -1.8660812E-02 -1.8660812E-02	2.3275860E-02 5.0595306E-02 2.7410756E-02 -2.7410756E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -2.3007837E-02 -1.4273564E-02 -1.4273564E-03 -4.2282845E-03 -1.4766257E-03 -2.5546250E-03 -1.4766257E-03 -2.3546250E-04 -1.200306E-04 -3.0252716E-05 2.3357655E-06 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -7.8782411E-07 2.7452198E-07 -7.9553252E-08 -4.6168113E+01 -4.6168113E+01 -4.542468E-03 1.6870164E-04 -3.7507757E-04 -1.0027874E-03 1.4554968E-03 -1.9025030E-03 2.3062452E-03 -7.9029406E-03 -1.1019740E-01 -5.4657109E-01 1.3351790E-01 1.5.4557109E-01 1.3351790E-01 -5.4657109E-01 -5.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.4657109E-01 -3.495937E-02 -7.0874802E-02 -3.8920165E-02 -1.9500814E-02 -1.9500814E-02 -1.9500814E-02	1.5984258E-02 3.1409317E-02 -2.4170697E-03 -1.0252173E-02 -1.2529869E-02 -1.2529869E-02 -1.2529869E-03 -3.4955699E-03 -2.1893129E-03 -3.4955699E-03 -2.1893129E-03 -1.3236088E-03 -7.6444915E-04 -4.1927555E-04 -2.1018932E-04 -2.1018932E-04 -2.00465586E-05 -1.2655586E-05 -1.2655586E-05 -1.2056324E-06 -4.0646724E-07 -4.1038958E-08 -2.0416597E-05 -7.1672253E-05 -2.0535337E-04 -2.7390373E-04 -4.9867871E-04 2.6902937E-03 2.9228815E-02 2.8313912E-01 -4.5481993E-01 -4.5481993E-01 -4.8407881E-01 -4.5481993E-01 -2.04978E-01 -2.04978E-01 -2.04978E-02 -2.4979948E-01 -2.04978E-01 -2.04978E-02 -2.4979948E-01 -2.049797E-02 -3.4056843E-02 -1.8638224E-02 -3.4056843E-02 -1.8638224E-02 -3.4056843E-03 -4.6416309E-03	8.6821874E-03 1.6152076E-02 8.3130239E-03 -1.2082964E-03 -5.4284824E-03 -6.1904548E-03 -3.1518739E-03 -3.8340378E-03 -2.6224758E-03 -1.7203202E-03 -1.7762097E-03 -3.7581084E-04 -2.0623615E-04 -3.7581084E-04 -2.0623615E-04 -4.3308889E-05 -7.6940850E-06 5.9103384E-07 -1.9917466E-07 -6.9388206E-08 -2.0107018E-08 -2.6310064E-04 -5.6527686E-05 -6.1665581E-03 -3.6031104E-02 -2.4163851E-01 -3.3603104E-02 -2.4163851E-01 -2.2464671E-01 -1.32477329E-01 4.3905387E-01 1.541172E-01 -2.2646971E-01 2.166347E-01 1.5892391E-02 -2.46651E-02 -8.4760406E-03 -1.900748E-02 -1.4050746E-02 -1.4050746E-02 -1.4050746E-02 -1.4050746E-02 -1.4050746E-02 -1.4050746E-02 -1.4050746E-02 -1.4050746E-03 -1.900438E-03 -1.9006388E-03 -1.9005382E-01	3.8967421E-03 7.2202503E-03 3.6937536E-03 -5.2904485E-04 -2.3988415E-03 2.7322183E-03 -2.2742441E-03 -1.6916478E-03 -7.5897747E-04 -4.7486954E-04 -1.6581658E-04 -9.0988010E-05 -4.5593595E-05 -4.5593595E-05 -1.9107141E-05 -3.3949229E-06 2.608264E-07 -8.7921529E-08 3.0630487E-08 -8.8759999E-09	1.1925690E-03 2.2172770E-03 1.1306051E-03 -1.6088394E-04 -7.3499143E-04 -8.3610751E-04 -8.3610751E-04 -2.3230106E-04 -1.4537414E-04 -3.5430612E-04 -3.5430612E-04 -2.7850367E-05 -3.8484891E-06 -1.0393242E-06 -1.0393242E-06 -2.6392237E-08 9.3829787E-09 -2.7189798E-09

198	1.5571453E+04	1.8505689E-02	-9.7166701E-03	-5.0445737E-03	-2.4093916E-03	-9.9205398E-04
199	3.4144729E+04	1.0053157E-02	-5.2431315E-03	-2.7184682E-03	-1.2973726E-03	-5.3378266E-04
200	7.7552073E+04	5.7074514E-03	-2.9660586E-03	-1.5361338E-03	-7.3311748E-04	-3.0174582E-04
201	1.8331766E+05	3.2157856E-03	-1.6675210E-03	-8.6327145E-04	-4.1187645E-04	-1.6947378E-04
202	4.5318823E+05	1.8747197E-03	-9.7110390E-04	-5.0256289E-04	-2.3978410E-04	-9.8678508E-05
203	1.1774969E+06	1.0050904E-03	-5.2031431E-04	-2.6924530E-04	-1.2845081E-04	-5.2855503E-05
204	3.2312090E+06	5.6000966E-04	-3.0010914E-04	-1.5551049E-04	-7.4096326E-05	-3.0491304E-05
205	2 0216802E+07	1 /083690E-04	-7.2866088E-05	-0.0108171E-05	-3.1300074E-05	-7.4010218E-06
200	2.32100321.07	1.40030301 04	1.20000001 03	5.1033203E 05	1.79000000 00	7.40102105 00
201						
208	1.9453737E-02	-6.3405875E-06	-2.1301527E-08	1.0700958E-06	1.1834573E-07	-1.4440979E-07
210	3.6141658E-02	3.1756298E-06	-6.2079715E-08	-3.0754875E-07	2.5434252E-08	-1.7462909E-07
211	6.7145353E-02	-1.0272372E-05	1.8208140E-07	1.0384013E-06	-1.7584224E-07	-1.2767581E-05
212	1.2474818E-01	-2.8077997E-06	-5.9212891E-07	2.3316708E-06	7.8600651E-07	-1.0380398E-04
213	2.3178217E-01	-1.4868391E-05	1.1352799E-06	-1.2643904E-06	-1.5375906E-06	-9.4873522E-04
214	4.3071120E-01	-1.6397545E-05	-2.5374135E-06	1.0584723E-05	1.4608141E-05	-2.8579440E-03
215	8.0058681E-01	-3.0646694E-05	4.5490830E-06	-8.3293775E-06	2.1429967E-04	-3.1528512E-03
216	1.4887931E+00	-4.6806616E-05	-9.3651340E-06	3.0953812E-05	2.8198685E-03	1.3426030E-03
217	2.7707233E+00	-7.4042998E-05	1.5121921E-05	-9.3897732E-05	9.3362928E-03	6.6422439E-03
218	5.1625848E+00	-1.2240603E-04	-3.0538176E-05	-2.0241203E-03	5.8098961E-03	3.9909902E-03
219	9.6361639E+00	-1.8777740E-04	9.6634033E-05	-1.3818484E-02	-1.2248394E-02	-5.7314004E-03
220	1.8031447E+01	-3.2211346E-04	1.5905883E-03	-1.9458426E-02	-1.5710492E-02	-7.3093403E-03
221	3.3858337E+01	-4.7314779E-04	1.5261706E-02	6.4268708E-03	2.0740600E-03	7.8182821E-04
222	6.3875692E+01	-1.4529518E-04	3.4917787E-02	2.9967022E-02	1.6249261E-02	6.8487906E-03
223	1.21251//E+02	8.2853578E-03	2.0507632E-02	1.7060952E-02	9.1405048E-03	3.8/233/3E-03
224	2.3200920E+02	3.2555/35E-02	-1.2945668E-02	-5.5915260E-03	-2.52/0209E-03	-1.03636/3E-03
220	4.40401/5E+02	5 0500227E 00	-3.04928/8E-02	-1.0290141E-02	-7 4207210E 02	-3.210/218E-03
220	1 7450942E+03	3 7447604E-02	-2.9100109E-02	-1.0964739E-02	-7.4297312E-03	-2.1611221E-03
228	3 5348455F+03	2 3852880F-02	-1 2946615E-02	-6 7744329F-03	-3 2432913E-03	-1 3367386F-03
229	7,3220404E+03	1.4124865E-02	-7.5432175E-03	-3.9350911E-03	-1.8801817E-03	-7,7334285E-04
230	1.5571453E+04	8.0835488E-03	-4.2798586E-03	-2.2258142E-03	-1.0638691E-03	-4.3828285E-04
231	3.4144729E+04	4.5718285E-03	-2.4029105E-03	-1.2485434E-03	-5.9598784E-04	-2.4511095E-04
232	7.7552073E+04	2.5752205E-03	-1.3482502E-03	-6.9931356E-04	-3.3399060E-04	-1.3755417E-04
233	1.8331766E+05	1.4456696E-03	-7.5366895E-04	-3.9079113E-04	-1.8646403E-04	-7.6690789E-05
234	4.5318823E+05	8.0607364E-04	-4.1939263E-04	-2.1722188E-04	-1.0369475E-04	-4.2695616E-05
235	1.1774969E+06	4.3778461E-04	-2.2721593E-04	-1.1767658E-04	-5.6138179E-05	-2.3091594E-05
236	3.2312890E+06	2.3188841E-04	-1.2025115E-04	-6.2238374E-05	-2.9702038E-05	-1.2227164E-05
237	9.4102964E+06	1.0715191E-04	-5.5493574E-05	-2.8723429E-05	-1.3701658E-05	-5.6364792E-06
238	2.9216892E+07	4.8678287E-05	-2.5204121E-05	-1.3040938E-05	-6.2224697E-06	-2.5611349E-06
239						
240						
241		2P+	3P+	4P+	5P+	6P+
242		-0.1939659E+02	-1.5549253E+02	-3.8038859E+01	-/./22825/E+00	-9.54/8329E-01
9.4.9						
243						
$243 \\ 244 \\ 245$	1 9453737F-02	1 79097685-06	-1 735781/F-05	1 14784985-05	2 3943494E-05	2 98570625-04
243 244 245 246	1.9453737E-02	1.7909768E-06	-1.7357814E-05	1.1478498E-05	2.3943494E-05 -7 7232160E-05	2.9857062E-04
243 244 245 246 247	1.9453737E-02 3.6141658E-02 6.7145353E-02	1.7909768E-06 -6.9040715E-06 1.5412243E-05	-1.7357814E-05 6.6855639E-05 -1.4884694E-04	1.1478498E-05 -4.3412352E-05 9.7117396E-05	2.3943494E-05 -7.7232160E-05 2.4491676E-04	2.9857062E-04 1.4984484E-03 1.5742169E-02
243 244 245 246 247 248	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04	1.1478498E-05 -4.3412352E-05 9.7117396E-05 -1.5994485E-04	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01
243 244 245 246 247 248 249	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04	1.1478498E-05 -4.3412352E-05 9.7117396E-05 -1.5994485E-04 2.4000122E-04	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01
243 244 245 246 247 248 249 250	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -6.3065591E-05	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04	1.1478498E-05 -4.3412352E-05 9.7117396E-05 -1.5994485E-04 2.4000122E-04 -3.3728483E-04	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04 -5.5370295E-03	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 5.3672586E-01
243 244 245 246 247 248 249 250 251	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -6.3065591E-05 9.0321565E-05	-1.7357814E-05 6.8855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 -8.4149659E-04	1.1478498E-05 -4.3412352E-05 9.7117396E-05 -1.5994485E-04 2.4000122E-04 -3.3728483E-04 2.6508045E-04	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 5.3672586E-01 2.4351525E-01
243 244 245 246 247 248 249 250 251 252	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E+00	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -6.3065591E-05 9.0321565E-05 -1.2406804E-04	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 -8.414965BE-04 1.1748943E-03	1.1478498E-05 -4.3412352E-05 9.7117396E-05 -1.5994485E-04 2.4000122E-04 -3.3728483E-04 2.6508045E-04 3.8248978E-04	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 5.3672586E-01 2.4351525E-01 -2.9947901E-01
243 244 245 246 247 248 249 250 251 252 253	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E+00 2.7707233E+00	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -6.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 5.9706844E-04 1.1748943E-03 -1.3762562E-03	1.1478498E-05 -4.3412352E-05 9.7117396E-05 2.4000122E-04 -3.3728483E-04 2.6508045E-04 3.8248978E-04 1.6246402E-02	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6832060E-01 2.435152E-01 2.9437901E-01 -4.3831897E-01
243 244 245 246 247 248 249 250 251 252 253 253 253	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E+00 2.7707233E+00 5.1625848E+00	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -6.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 -2.2496858E-04	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 -8.4149659E-04 1.1748943E-03 -1.3762562E-03 1.8294319E-03	1.1478498E-05 -4.3412352E-05 9.7117396E-05 -1.599445E-04 -3.3728483E-04 2.600122E-04 3.8248978E-04 1.6246402E-02 2.1741344E-01	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.4410348E-02	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 2.435152E-01 2.9947901E-01 -4.3831897E-01 -4.3831897E-01
243 244 245 246 247 248 249 250 251 252 253 254 255 255	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 8.0058681E-01 1.4887931E+00 0.77707233E+00 5.1625848E+00 9.6361639E+00	1.7909768E-06 -6.9040715E-06 -2.7149733E-05 -2.7149733E-05 -6.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 -2.2496658E-04 2.4499503E-04	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 -8.4149659E-04 1.1748943E-03 -1.3762562E-03 1.8294319E-03 -7.7437667E-03	1.1478498E-05 -4.3412352E-05 9.7117396E-05 -1.5994455E-04 2.4000122E-04 -3.3728463E-04 2.6508045E-04 3.8248978E-04 1.6264002E-02 2.1741344E-01 6.5460596E-01	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 5.3672586E-01 2.4351525E-01 -2.9947901E-01 -4.3831897E-01 -4.3831897E-01 -4.9284966E-02 2.6628797E-01
243 244 245 246 247 248 249 250 251 252 253 254 255 256 255	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 1.4887931E+00 2.7707233E+00 5.1625848E+00 9.6361639E+00 1.8031447E+01 2.926927E-01	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149738E-05 -6.3065591E-05 -0.321565E-05 -1.2406804E-04 1.8019397E-04 -2.2496858E-04 -2.4499503E-04 -4.6779083E-04	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 8.4149659E-04 1.1748943E-03 -1.3762562E-03 1.8294319E-03 -7.7437667E-03 -1.0330252E-01	1.1478498E-05 -4.3412352E-05 9.7117396E-05 1.5994485E-04 2.4000122E-04 -3.3728483E-04 2.6508045E-04 3.8248978E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 3.8926786E-01	2.3943494E-05 -7.7232160E-05 2.4491676E-04 4.2.4121140E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01 3.0640830E-01 1.72000E-01	2.9857062E-04 1.4984484E-03 1.5742169E-02 3.6830260E-01 5.3672586E-01 -2.93672586E-01 -2.9347901E-01 -4.3831897E-01 -4.9284966E-02 2.6628797E-01 1.3425171E-01
243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 1.4887931E-00 2.7707233E+00 5.1625848E+00 9.6361638E+00 1.8031447E+01 3.3858337E+01 3.3858337E+01	1.7909768E-06 -6.9040715E-06 1.5412243E-05 2.7149738E-05 4.2620264E-05 -6.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 -2.2496858E-04 2.4499503E-04 -4.6779083E-04 1.0638953E-03 2.9677068E-02	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 -1.1748943E-03 -1.3762562E-03 1.8294319E-03 -7.7437667E-03 -7.7437667E-03 -1.0330252E-01 -4.4550532E-01	1.1478498E-05 -4.3412352E-05 9.7117396E-05 2.4000122E-04 -3.3728438E-04 2.6508045E-04 3.824878E-04 1.6246402E-02 2.1741344E-01 3.8926786E-01 -3.4215046E-01 -3.4215046E-01	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-01 -6.8213430E-01 -4.410348E-02 5.9530979E-01 3.0640830E-01 -1.7300060E-01	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 2.4351525E-01 2.4351525E-01 -4.9847901E-01 -4.984966E-02 2.6628797E-01 1.3425171E-01 -6.9214175E-02 9.40560502E-02
243 244 245 246 247 248 249 250 251 252 253 254 255 255 255 255 257 258 259	1.9453737E-02 3.6141658E-02 6.7145358-02 1.2474818E-01 2.3178217E-01 8.0058661E-01 1.4887931E+00 0.7707238E+00 9.6361639E+00 1.6051447E+01 3.8858337E+01 6.3875692E+01 1.2125177E+02	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -6.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 -2.249658E-04 2.4499503E-04 1.0638953E-03 2.9507066E-02 1.8226800E-01	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 -8.4149659E-04 1.1748943E-03 -1.3762562E-03 1.8294319E-03 -7.7437667E-03 -1.0330252E-01 -4.4550532E-01 -5.0175633E-01 -6.938297E-02	1.1478498E-05 -4.3412352E-05 9.7117396E-05 2.4000122E-04 -3.3728483E-04 2.6508045E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 -3.8226786E-01 -3.4215046E-01 -4.3575268E-01	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 -3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01 3.0640830E-01 -1.7300060E-01 -2.3448067E-01 -4.4661336E-02	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6832050E-01 2.435152E-01 2.9347901E-01 -4.3831897E-01 -4.9284966E-02 2.6628797E-01 1.3425171E-01 -6.9214175E-02 -9.4050509E-02 1.7339228E-02
$\begin{array}{c} 243\\ 244\\ 245\\ 246\\ 247\\ 248\\ 249\\ 250\\ 251\\ 252\\ 253\\ 254\\ 255\\ 256\\ 257\\ 258\\ 259\\ 260\\ \end{array}$	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 8.0058681E-01 1.4887931E+00 0.77707233E+00 5.1625848E+00 9.6361639E+00 1.8031447E+01 6.3875692E+01 1.2125177E+02 2.320092E+02	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -0.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 -2.249688E-04 2.4499503E-04 -4.6779083E-03 2.9507066E-02 1.8226800E-01 3.4067653E-01	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 1.7748943E-03 -1.3762562E-03 -1.3762562E-03 -7.7437667E-03 -1.0330252E-01 -4.4550532E-01 -5.0175633E-01 -6.9382970E-02 1.9950681E-01	1.1478498E-05 -4.3412352E-05 9.711736E-05 1.599445E-04 2.4000122E-04 -3.3728463E-04 2.6508045E-04 3.8248978E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 3.8926766E-01 -3.4215046E-01 -4.3575268E-01 -7.7621230E-02	2.3943494E-05 -7.7232160E-05 2.4491676E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01 3.0640830E-01 -1.730060E-01 -2.3448067E-01 -4.9759817E-02	2.9857062E-04 1.4984484E-03 1.5742169E-02 3.6830260E-01 5.3672586E-01 -2.9947901E-01 -4.3831897E-01 -4.9284666E-02 2.6628797E-01 1.3425171E-01 -6.9214175E-02 -9.4050509E-02 -1.7339228E-02
$\begin{array}{c} 243\\ 244\\ 245\\ 246\\ 247\\ 248\\ 249\\ 250\\ 251\\ 252\\ 253\\ 254\\ 255\\ 256\\ 257\\ 258\\ 259\\ 260\\ 261\\ \end{array}$	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 1.4887931E+00 2.7707233E+00 0.536638E+00 9.6361639E+00 1.8031447E+01 1.3858337E+01 6.3875692E+01 1.2125177E+02 2.3200920E+02 4.848175E+02	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149738E-05 -2.7149738E-05 -4.2620264E-05 -1.2406804E-04 1.8019397E-04 -2.2496858E-04 -2.2496858E-04 -2.4499503E-04 1.0638953E-03 2.9507066E-02 1.8226800E-01 3.4067653E-01 3.0831828E-01	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 8.4149659E-04 1.1748943E-03 -1.3762562E-03 -7.7437667E-03 -7.7437667E-03 -1.0330252E-01 -6.9382970E-02 1.9950681E-01 1.9261829E-01	1.1478498E-05 -4.3412352E-05 9.7117396E-05 1.5994485E-04 2.4000122E-04 -3.3728483E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 3.8228778E-01 -3.4215046E-01 -4.3575268E-01 -7.7621230E-02 1.0498458E-01	2.3943494E-05 -7.7232160E-05 2.4491676E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01 3.0640830E-01 -1.730060E-01 -2.3448067E-01 -4.2661336E-02 4.9759817E-02 5.0149212E-02	2.9857062E-04 1.4984484E-03 1.5742169E-02 3.6830260E-01 5.3672586E-01 -2.9547901E-01 -4.9381897E-01 -4.9284966E-02 2.6628797E-01 1.3425171E-01 -9.4050509E-02 -9.4050509E-02 -1.7339228E-02 1.9538359E-02
$\begin{array}{c} 243\\ 244\\ 245\\ 246\\ 247\\ 248\\ 249\\ 250\\ 251\\ 252\\ 253\\ 254\\ 255\\ 256\\ 257\\ 258\\ 259\\ 260\\ 261\\ 262\\ \end{array}$	1.9453737E-02 3.6141658E-02 6.7146338-02 6.714533E-01 2.3178217E-01 4.3071120E-01 4.3071120E-01 1.4887931E-00 2.7707233E+00 9.6361639E+00 1.8031447E+01 3.3858337E+01 1.2125177E+02 2.3200920E+02 4.7781809E+02	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149738E-05 -2.7149738E-05 -1.2406804E-04 1.8019397E-04 -2.249658E-04 2.4499503E-04 1.6633953E-03 2.9507066E-02 1.8226800E-01 3.0831828E-01 1.7951817E-01	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -2.0157013E-04 -4.0809632E-04 5.9706844E-04 -1.1748943E-03 -1.3762562E-03 -7.7437617E-03 -7.7437617E-03 -1.0330252E-01 -4.4550532E-01 -5.0175633E-01 -6.9382970E-02 1.9950681E-01 1.9261829E-01 1.0697797E-01	1.1478498E-05 -4.3412352E-05 9.7117396E-05 2.4000122E-04 -3.3728483E-04 2.6508045E-04 3.8248978E-04 1.6246402E-02 2.1741344E-01 3.8926786E-01 -3.4215046E-01 -7.7621230E-02 1.0498458E-01 1.0475926E-01 5.7260854E-02	2.3943494E-05 -7.7232160E-05 2.4491676E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.410348E-02 5.953079E-01 3.0640830E-01 -1.7300060E-01 -2.3448067E-01 -2.3448067E-01 -4.2661336E-02 5.0149212E-02 2.7288808E-02	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 2.4351525E-01 -2.9947901E-01 -4.9381897E-01 1.3425171E-01 -6.9214175E-02 9.4050509E-02 -1.7339228E-02 1.968628E-02 1.968628E-02 1.070897E-02
243 244 245 246 247 250 251 252 253 254 255 256 257 258 259 260 261 262 263	1.9453737E-02 3.6141658E-02 6.7145358E-02 1.2474818E-01 2.3178217E-01 8.0058681E-01 1.4887931E+00 9.6361639E+00 9.6361639E+00 1.8031447E+01 3.3858337E+01 6.3875692E+01 1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.74510942E+03	1.7909768E-06 -6.9040715E-06 -2.7149733E-05 4.2620264E-05 -0.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 -2.2496858E-04 2.4499503E-04 1.0633953E-03 2.9507066E-02 1.8226800E-01 3.4067653E-01 1.7951817E-01 8.1558104E-02	-1.7357814E-05 6.685639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 -8.4149659E-04 1.748943E-03 -1.3762562E-03 -1.7437667E-03 -1.030252E-01 -4.4550532E-01 -6.9382970E-02 1.9950681E-01 1.99261829E-01 1.0697797E-01 4.6333840E-02	1.1478498E-05 -4.3412352E-05 9.7117396E-05 2.4000122E-04 -3.3728483E-04 2.6508045E-04 2.6508045E-04 3.8248978E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 -3.4215046E-01 -3.4215046E-01 -7.7621230E-02 1.0498458E-01 1.0475926E-01 5.7260854E-02 2.4943775E-02	2.3943494E-05 -7.7232160E-05 2.4491676E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 4.2661051E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01 3.0640830E-01 -1.7300060E-01 -2.3448067E-01 -4.266135E-02 4.9759817E-02 5.0149212E-02 2.7288808E-02 1.1869221E-02	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 2.435152E-01 2.947901E-01 -4.3831897E-01 -4.9284966E-02 2.6628797E-01 1.3425171E-01 -6.9214175E-02 -9.405609E-02 1.7339228E-02 1.9538359E-02 1.9588628E-02 1.0708997E-02 4.6482124E-03
$\begin{array}{r} 243\\ 244\\ 245\\ 246\\ 247\\ 248\\ 249\\ 250\\ 251\\ 252\\ 253\\ 254\\ 255\\ 256\\ 257\\ 258\\ 259\\ 260\\ 261\\ 262\\ 263\\ 264\\ \end{array}$	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 8.0058681E-01 1.4887931E+00 2.7707233E-00 9.6361639E+00 1.602848E+00 9.6361639E+00 1.8031447E+01 6.3875692E+01 1.2125177E+02 8.7781809E+02 1.7450942E+03 3.534455E+03	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -0.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 2.249658E-04 2.4499503E-04 -4.6779063E-04 1.0638953E-03 2.9507066E-02 1.8226800E-01 3.4067653E-01 3.0831828E-01 1.7951817E-01 8.1558104E-02 3.1965643E-02	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 1.1748943E-03 -1.3762562E-03 -7.7437667E-03 -7.7437667E-03 -7.7437667E-03 -1.0330252E-01 -5.0175633E-01 -6.9382970E-02 1.9950681E-01 1.99516829E-01 1.6697797E-01 1.6693797E-01 1.765602E-02	1.1478498E-05 -4.3412352E-05 9.7117396E-05 1.5994485E-04 2.4000122E-04 -3.3728463E-04 2.6500465E-04 3.8248978E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 3.8926786E-01 -3.4215046E-01 -3.4215046E-01 -7.7621230E-02 1.049848E-01 1.0475926E-01 5.7260854E-02 2.4943775E-02 9.4703531E-03	2.3943494E-05 -7.7232160E-05 2.4491676E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01 3.0640830E-01 -2.3448067E-01 -2.3448067E-01 -4.975817E-02 5.0149212E-02 4.975817E-02 5.0149212E-02 1.1869221E-02 4.4956032E-03	2.9857062E-04 1.4984484E-03 1.5742169E-02 3.6830260E-01 5.3672586E-01 -2.9947901E-01 -4.3831897E-01 -4.9284966E-02 2.6628797E-01 1.3425171E-02 -9.4050509E-02 -1.7339228E-02 1.9558358E-02 1.955859E-02 1.955859E-02 1.9558528E-02 1.9558528-03 1.7627458E-03 1.7627458E-03
$\begin{array}{r} 243\\ 244\\ 245\\ 246\\ 247\\ 248\\ 249\\ 250\\ 251\\ 252\\ 253\\ 255\\ 256\\ 257\\ 258\\ 259\\ 260\\ 261\\ 262\\ 263\\ 264\\ 265\\ \end{array}$	1.9453737E-02 3.6141658E-02 2.3178217E-01 4.3071120E-01 1.4887931E+00 2.7707233E+00 2.7707233E+00 0.6361639E+00 1.8031447E+01 1.3858337E+01 6.3875692E+01 1.2125177E+02 4.848175E+02 8.7781809E+02 1.7450942E+03 3.534465E+03 7.3220404E+03	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149738E-05 -2.7149738E-05 -4.2620264E-05 -1.2406804E-04 1.8019397E-04 -2.2496858E-04 2.4499503E-04 1.6638953E-03 2.9507066E-02 1.8226800E-01 3.4067653E-01 3.0831828E-01 1.7951817E-01 8.1558104E-02 3.1965643E-02 1.1545310E-02	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 8.4149659E-04 1.1748943E-03 -7.7437667E-03 -7.7437667E-03 -1.0330252E-01 -6.9382970E-02 1.9950681E-01 1.9261829E-01 1.0697797E-01 4.6938340E-02 1.7965602E-02 6.4093369E-03	1.1478498E-05 -4.3412352E-05 9.7117396E-05 1.5994485E-04 2.4000122E-04 -3.3728433E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 3.8926786E-01 -3.4215046E-01 -3.4215046E-01 -7.7621230E-02 1.0498458E-01 1.0475926E-01 5.7260854E-02 2.4943775E-02 2.4943775E-02 9.4703531E-03 3.3749812E-03	2.3943494E-05 -7.7232160E-05 2.4491676E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -4.4410348E-02 5.9530979E-01 3.0640830E-01 -1.7300060E-01 -2.3448067E-01 -2.3448067E-01 -2.3448067E-01 -2.348067E-01 -2.3480867E-01 -4.2661336E-02 4.9759817E-02 2.7288808E-02 1.1869221E-02 1.6022521E-03	2.9857062E-04 1.4984484E-03 1.5742169E-02 3.6830260E-01 5.3672586E-01 -2.9347901E-01 -4.9381997E-01 1.3425171E-01 -9.4050508E-02 2.6628797E-01 1.3425171E-01 -9.4050508E-02 -1.7339228E-02 1.9583859E-02 1.9583859E-02 1.965828E-02 1.0708997E-02 4.6482124E-03 1.7627453E-03 6.2708462E-04
243 244 245 246 247 248 250 250 255 255 255 255 255 255 255 255	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 1.4387931E-00 2.7707233E+00 9.6361639E+00 1.8031447E+01 3.3568337E+01 1.2125177E+02 2.3200920E+02 4.748507E+02 1.7450942E+03 3.5348455E+03 7.3220404E+03 1.5571453E+04	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.714973E-05 4.2620264E-05 -6.3065591E-05 -1.2406804E-04 1.8019397E-04 -2.249658E-04 2.4499503E-04 1.0638953E-03 2.9507066E-02 1.8226800E-01 3.0831828E-01 1.7951817E-01 8.1558104E-02 3.1965643E-02 1.1545310E-02 3.9616034E-03 	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 1.1748943E-03 -1.3762562E-03 1.8294319E-03 -7.7437667E-03 -7.7437667E-03 -1.0330252E-01 -6.9382970E-02 1.9950681E-01 1.9261829E-01 1.9261829E-01 1.0697797E-01 4.693340E-02 1.7965602E-02 6.4093369E-03 2.1806178E-03	1.1478498E-05 -4.3412352E-05 9.7117396E-05 2.4000122E-04 -3.3728483E-04 2.6508045E-04 3.8248978E-04 1.6246402E-02 2.1741344E-01 3.8926786E-01 -3.4215046E-01 -3.4215046E-01 1.0475926E-01 5.7260854E-02 2.4943775E-02 9.470351E-03 3.3749812E-03 1.1431679E-03	2.3943494E-05 -7.7232160E-05 2.4491676E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-01 -6.8213430E-01 -4.461051E-01 -6.8213430E-01 -4.410348E-02 5.953079E-01 3.0640830E-01 -1.7300060E-01 -2.3448067E-01 -4.2661336E-02 4.9759817E-02 5.0149212E-02 5.0149212E-02 1.1869221E-02 1.6022521E-03 5.4188309E-04	2.9857062E-04 1.4984484E-03 1.5742169E-02 1.0098719E-01 3.6830260E-01 2.4351525E-01 2.943701E-01 -4.984390E-02 2.6628797E-01 1.3425171E-01 -6.9214175E-02 9.4056059CE-02 1.7339228E-02 1.9583628E-02 1.070897E-02 4.6422124E-03 1.7627452E-03 1.7627452E-03 1.7627452E-04 2.1244923E-04
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243 244 245 246 247 248 248 248 250 251 252 255 256 257 258 259 260 261 262 263 264 265 266 266 267 264 265 264 265 264 265 264 265 264 265 264 277 273 273 274 277 273 273 274 275 275 268 269 270 271 272 283 274 275 273 274 275 275 268 269 270 271 272 273 273 274 275 275 275 268 269 270 271 272 273 274 275 275 275 275 275 275 275 275 275 275	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 8.0058681E-01 1.4887931E+00 2.7707233E+00 9.6361639E+00 1.605848E+00 9.6361639E+00 1.83875692E+01 1.2125177E+02 8.7781809E+02 1.7450942E+03 3.534455E+03 7.322040E+03 3.534455E+03 7.322040E+03 3.534455E+04 3.51453E+04 3.512862E+05 1.1774969E+06 3.2312800E+06 9.4102964E+06 2.9216892E+07 1.9453737E-02 3.6141658E+02 3.178217E+01 2.3178217E+01 3.1782737E+02 3.6141658E+02 3.178217E+01 2.3178217E+01 3.31782E+07 3.6141658E+02 3.178232E+07 1.9453737E+02 3.6141658E+02 1.2474818E+01 2.3178217E+01 3.058681E+01 1.4887931E+00 2.707233E+00 5.1625848E+00 9.6361639E+00 1.8031447E+01 3.3856337E+01	1.7909768E-06 -6.9040715E-06 1.5412243E-05 -2.7149733E-05 4.2620264E-05 -0.3065591E-05 9.0321565E-05 -1.2406804E-04 1.8019397E-04 2.249658E-04 2.4499503E-04 -2.249658E-04 2.4499503E-04 1.638953E-03 2.9507066E-02 1.8226800E-01 3.0831828E-01 1.7951817E-01 8.1558104E-02 3.9616034E-03 1.3204201E-03 4.3643664E-05 1.3360438E-05 1.3360438E-06 3.6303539E-07 8.5985209E-10 -6.601057E-09 8.5985209E-10 -6.63775406E-08 1.4544617E-07 -3.061793E-07 6.158537E-07 -1.1769394E-06 2.372425E-06 -4.0748728E-06 2.372425E-06 -1.6058505E-05 5.0629269E-05	-1.7357814E-05 6.6855639E-05 -1.4884694E-04 2.6157013E-04 -4.0809632E-04 5.9706844E-04 1.1748943E-03 -1.3762562E-03 -7.7437667E-03 -1.330252E-01 1.8294319E-03 -7.7437667E-03 -1.0330252E-01 1.9950681E-01 1.9950681E-01 1.995602E-02 6.4093369E-03 2.1806178E-03 7.2399824E-04 2.3691871E-05 7.2447862E-06 2.1845507E-06 2.1845507E-08 1.3488641E-07 1.9603153E-07 -2.8531377E-08 1.3488641E-07 -3.8144270E-07 8.6999191E-07 -1.7872119E-06 3.4765381E-06 -3.87616E-06 1.936022E-05 -1.9845084E-04 -3.5882024E-03 -2.1201098E-02	1.1478498E-05 -4.3412352E-05 9.7117396E-05 1.5994485E-04 2.4000122E-04 -3.3728483E-04 1.6246402E-02 2.1741344E-01 6.5460596E-01 3.4215046E-01 -3.4215046E-01 -4.3575268E-01 -7.7621230E-02 1.0498458E-01 1.0475926E-01 5.7260854E-02 2.4943775E-02 9.4703531E-03 3.3749812E-03 3.3749812E-03 3.8013189E-04 1.2289346E-04 3.9519284E-02 3.7964614E-06 1.1390236E-06 2.9927507E-07 1.0213144E-07 -3.7850697E-07 8.15760424E-07 -3.7850697E-07 8.15780424E-07 -3.7850697E-07 8.15780424E-07 -3.7850697E-07 1.0213144E-09 -4.4891603E-08 1.6483973E-06 2.2018911E-04 4.0345279E-03 1.6483775E-02 1.3464819E-02 -1.6269013E-02	2.3943494E-05 -7.7232160E-05 2.4491676E-04 -2.4121140E-04 3.2527832E-04 -5.5370295E-03 -7.4346300E-02 -4.2661051E-01 -6.8213430E-01 -1.7300060E-01 -2.3448067E-01 -2.3448067E-01 -2.3448067E-01 -2.3448067E-01 -2.3448067E-02 2.7288808E-02 1.169221E-02 2.728808E-02 1.6022521E-03 5.4183309E-04 1.833013E-04 5.8573101E-06 1.8004317E-06 5.3906370E-07 1.4197777E-07 4.8322849E-08 2.2295759E-08 -1.0228987E-07 -6.3081234E-07 1.1769234E-06 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.9500368E-05 -5.4304212E-04 -2.950368E-05 -5.4304212E-04 -2.950368E-05 -5.4304212E-04 -2.950368E-05 -5.4304212E-04 -2.950368E-05 -5.4304212E-04 -2.950368E-05 -5.4304212E-04 -2.950368E-05 -5.4304212E-04 -2.950368E-05 -5.4304212E-04 -5.29256E-03 -5.29256E-03 -5.29256	2.9857062E-04 1.4984484E-03 1.5742169E-02 3.6830260E-01 5.3672586E-01 -2.9947901E-01 -3.4351525E-01 -2.9947901E-01 -4.9284966E-02 2.6628797E-01 1.3425171E-01 -6.9214175E-02 -9.4050509E-02 1.9538359E-02 1.9538259E-02 1.9538258E-02 1.9538258E-02 1.9628422E-04 2.124923E-04 2.2825835E-05 7.3308702E-06 2.28658E-05 7.3308702E-06 2.2965841E-06 7.0393529E-07 2.3126122E-06 3.3737755E-07 2.3326122E-06 3.3737755E-07 2.3326122E-06 3.3737755E-07 2.3326122E-06 3.3737755E-07 2.3326122E-06 3.3737755E-07 2.9104377E-04 1.446630E-03 2.91076808E-04 6.7421216E-03 -3.926206E-03
200	6 3875602E+01	1 05106085-03	-3 2650281E-02	-0 8007307F-00	-1 52108105-02	-6 10/103/F-03
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290	1 2125177E+02	1.9519098E-03	-5.2059201E-02	-2.829/39/E-02	-1.5219819E-02	-0.1041034E-03
202	2 3200920E+02	4 2504697F-02	2 4747700F-02	1 3022969F-02	6 1730569E-03	2 4238896F-03
203	4 4845175F+02	5 2751818F-02	3 2633957F-02	1 7711917F-02	8 4747501E-03	3 3217453E-03
294	8 7781809F+02	4 1993602F-02	2 4737198F-02	1 3204440F-02	6 2884236F-03	2 4674815E-03
295	1.7450942E+03	2.5938621E-02	1.4742301E-02	7.8113383E-03	3.7142919E-03	1.4542888E-03
296	3.5348455E+03	1.3675392E-02	7.5863835E-03	3.9858465E-03	1.8904523E-03	7.4119349E-04
207	7 3220404E+03	6 5/96213E-03	3 590/302E-03	1 8851858E-03	8 9/3771/F-0/	3 /002//55-0/
200	1.5220404E+03	0.0490213E-03	1 597140EE 02	1.0001000E_04	0.9437714E-04	1 F200420E 04
290	2 4144700E+04	2.9104044E-03	1.3871403E-03	2 E004200E-04	1 6610122E-04	1.5596450E-04
200	7 75500725-04	1.2313309E-03	0.0030029E-04	1 3060E01E 04	C 55007155 05	0.4944090E-05
300	7.7552073E+04	4.9178426E-04	2.6591115E-04	1.3860521E-04	6.5589/15E-05	2.5/344/6E-05
301	1.8331/66E+05	1.8/2/8/1E-04	1.0140133E-04	5.3170924E-05	2.5225700E-05	9.8532403E-06
302	4.5318823E+05	6./1/2912E-05	3.6241344E-05	1.884/394E-05	8.91068/1E-06	3.5009323E-06
303	1.1//4969E+06	2.2854770E-05	1.23//549E-05	6.5065854E-06	3.0902551E-06	1.204/168E-06
304	3.2312890E+06	7.2396045E-06	3.8984144E-06	2.0189998E-06	9.528/306E-07	3.7546967E-07
305	9.4102964E+06	2.1116140E-06	1.145/808E-06	6.0568/10E-0/	2.8834299E-07	1.1195682E-07
300	2.9216892E+07	6.0709444E-07	3.2630424E-07	1.6820133E-07	7.9223167E-08	3.132332/E-08
200						
309		3D-	4D-	5D-	6D-	
310		-1 3454997F+02	-2 8440237F+01	-4 0958645F+00	-1 9118266F-01	
311		1.34343376102	2.04402571101	4.03300431.00	1.91102006 01	
312						
313	1.9453737E-02	1 7089039E-06	-9.8760413E-06	2 7995910E-05	1 4932202E-02	
314	3.6141658E-02	-6.0185033E-06	3.4969254E-05	-1.1368619E-04	9.0689119E-02	
315	6 7145353E-02	1 2797964F-05	-7 2799441E-05	1 7505638E-04	2 1700399F-01	
316	1 2474818F-01	-2 1957719F-05	1 2433456F-04	-4 9191642F-04	3 0663088F-01	
317	2 3178217F-01	3 4032852E-05	-1 8495013E-04	-8 3400901E-04	3 1911490F-01	
210	4 3071100E-01	-4 9957107E-05	2 9206060E-04	-1 995010/15-04	2 2061/615-01	
310	8 00526218-01	7 149101/18-05	-2 7828710F-04	-1 3000124E-02	6 4324911E-01	
330	1 /2070212-01	-0 711070FF 05	2.1020/19E-04	-3 8040000E 01	-1 1001170E 01	
J∠U 201	1.400/931E+00	3.1110125E-U5	3.0001056E-05	-/ 800006FF 01	1.12011/UE-U1	
222	2.11U1233E+00	1.03091/9E-04	1.1210400E-02	-1.0203005E-01	1.01/9030E-U1	
322	5.1525848E+00	-1.2595221E-05	-1.53/5034E-01	-1.7055544E-01	-5.812/068E-02	
323	9.6361639E+00	2.86/91/0E-03	-4.3440372E-01	2.2451693E-01	5.6934617E-02	
324	1.8031447E+01	4.4723198E-02	-4.34/3355E-01	2.5425237E-01	6.6990629E-02	
325	3.3858337E+01	2.0918124E-01	-9.0538223E-02	6.8020582E-02	1.8184440E-02	
326	6.3875692E+01	3.6808534E-01	1.//19/62E-01	-7.2767881E-02	-1.8121532E-02	
327	1.2125177E+02	3.1529005E-01	1.8203443E-01	-8.0174035E-02	-2.0259119E-02	
328	2.3200920E+02	1.7091567E-01	9.9398001E-02	-4.3637462E-02	-1.1003657E-02	
329	4.4845175E+02	6.9494681E-02	3.9939466E-02	-1.7558094E-02	-4.4348522E-03	
330	8.7781809E+02	2.3873371E-02	1.3493698E-02	-5.8836773E-03	-1.4818314E-03	
331	1.7450942E+03	7.6257647E-03	4.2969254E-03	-1.8824352E-03	-4.7542439E-04	
332	3.5348455E+03	2.3509435E-03	1.3111106E-03	-5.6913149E-04	-1.4316013E-04	
333	7.3220404E+03	7.7673255E-04	4.3465144E-04	-1.9037934E-04	-4.8106375E-05	
334	1.5571453E+04	2.4819454E-04	1.3762045E-04	-5.9590324E-05	-1.4976820E-05	
335	3.4144729E+04	1.0097160E-04	5.6322678E-05	-2.4649097E-05	-6.2274833E-06	
336	7.7552073E+04	2.3593046E-05	1.3051841E-05	-5.6438896E-06	-1.4177230E-06	
337	1.8331766E+05	1.9141952E-05	1.0646356E-05	-4.6448722E-06	-1.1718580E-06	
338						
339						
340	1.9453737E-02	-2.3494679E-08	2.6208878E-09	4.6634915E-08	2.0101141E-05	
341	3.6141658E-02	-1.9322798E-08	6.5634513E-08	-1.9694197E-07	1.6643639E-04	
342	6.7145353E-02	-3.7623054E-08	-1.3504919E-07	4.5212975E-07	5.4281184E-04	
343	1.2474818E-01	-1.7982510E-07	4.7295761E-07	-1.6027518E-06	1.0454788E-03	
344	2.3178217E-01	-1.0906279E-07	-6.8682944E-07	-3.8029510E-06	1.4830538E-03	
345	4.3071120E-01	-8.6077940E-07	2.1426726E-06	-1.2615206E-04	1.4546706E-03	
346	8.0058681E-01	-6.0012341E-07	-1.6582379E-06	-1.1417297E-03	5.5549240E-04	
347	1.4887931E+00	-3.7513449E-06	2.5787163E-06	-4.5032764E-03	-1.3286172E-03	
348	2.7707233E+00	-3.9610437E-06	-2.7331159E-04	-7.7561746E-03	-2.5348380E-03	
349	5.1625848E+00	-1.2698453E-05	-3.3672176E-03	-3.7359314E-03	-1.2732659E-03	
350	9.6361639E+00	5.8900205E-05	-1.3005742E-02	6.7252198E-03	1.7056459E-03	
351	1.8031447E+01	1.7787270E-03	-1.7785899E-02	1.0400561E-02	2.7403220E-03	
352	3.3858337E+01	1.1643180E-02	-5.0457069E-03	3.7911647E-03	1.0135104E-03	
353	6.3875692E+01	2.8130069E-02	1.3583480E-02	-5.5843513E-03	-1.3909320E-03	
354	1.2125177E+02	3.2908758E-02	1.9024063E-02	-8.3813030E-03	-2.1179794E-03	
355	2.3200920E+02	2.4220728E-02	1.4094371E-02	-6.1882584E-03	-1.5604250E-03	
356	4.4845175E+02	1.3211997E-02	7.5954655E-03	-3.3396728E-03	-8.4360128E-04	
357	8.7781809E+02	5.9478115E-03	3.3626162E-03	-1.4658614E-03	-3.6912643E-04	
358	1.7450942E+03	2.3895830E-03	1.3480030E-03	-5.9112469E-04	-1.4935917E-04	
359	3.5348455E+03	8.7767933E-04	4.8937629E-04	-2.1203365E-04	-5.3281030E-05	
360	7.3220404E+03	3.1659229E-04	1.7794360E-04	-7.8319996E-05	-1.9834947E-05	
361	1.5571453E+04	1.0762715E-04	5.9443293E-05	-2.5514972E-05	-6.3839772E-06	
362	3.4144729E+04	3.8715731E-05	2.1846633E-05	-9.7070014E-06	-2.4699387E-06	
363	7.7552073E+04	1.1319909E-05	6.1760611E-06	-2.6064317E-06	-6.4670721E-07	
364	1.8331766E+05	5.6586060E-06	3.1874249E-06	-1.4152137E-06	-3.6001496E-07	
365						
366						
367		3D+	4D+	5D+	6D+	
368		-1.2828009E+02	-2.6929354E+01	-3.8109062E+00	-1.8232759E-01	
369						
370						
371	1.9453737E-02	-1.7210672E-06	7.3132785E-06	-2.7776140E-05	-1.9530883E-02	
372	3.6141658E-02	6.0569545E-06	-2.6038313E-05	1.1990627E-04	-1.0438260E-01	
373	6.7145353E-02	-1.2879308E-05	5.3836184E-05	-1.6720252E-04	-2.3373561E-01	
374	1.2474818E-01	2.2080100E-05	-9.2557207E-05	5.8753465E-04	-3.1566074E-01	
375	2.3178217E-01	-3.4204831E-05	1.3382386E-04	1.4429520E-03	-3.1354910E-01	
376	4.3071120E-01	5.0047368E-05	-2.2717258E-04	2.5351517E-02	-2.0760139E-01	
377	8.0058681E-01	-7.0646065E-05	2.1103922E-04	1.5247930E-01	-3.9034285E-02	
378	1.4887931E+00	9.8359381E-05	2.7872922E-04	4.0535099E-01	1.2157603E-01	
379	2.7707233E+00	-1.0556997E-04	2.1603697E-02	4.6918787E-01	1.4784763E-01	
380	5.1625848E+00	-4.9550393E-05	1.7560741E-01	1.2765354E-01	4.3641198E-02	
381	9.6361639E+00	-3.7085325E-03	4.5397419E-01	-2.4344193E-01	-6.0722751E-02	

382	1.8031447E+01	-5.3425366E-02	4.1453450E-01	-2.4127529E-01	-6.1822179E-02
383	3.3858337E+01	-2.2898645E-01	5.5727504E-02	-4.9313322E-02	-1.2973639E-02
294	6 207E600E+01	-2 76655645-01	-1 0097000E-01	7 04967945-00	1 0249004E-02
0.04	0.30/3092E+01	-3.7005504E-01	-1.900/229E-01	7.9400704E-02	1.93469046-02
385	1.2125177E+02	-3.0417809E-01	-1.7732290E-01	7.7728580E-02	1.9124179E-02
386	2.3200920E+02	-1.5582420E-01	-9.0941139E-02	3.9705444E-02	9.7488921E-03
387	4.4845175E+02	-5.9172363E-02	-3.4051989E-02	1.4873841E-02	3.6575156E-03
388	8.7781809E+02	-1.8361206E-02	-1.0392119E-02	4.5029277E-03	1.1039906E-03
280	1 74500405+02	-E 0202400E-02	-0 9410090E-02	1 00706505-00	2 04520195-04
309	1.74309426+03	-5.0293490E-03	-2.0410202E-03	1.2378039E-03	3.04520186-04
390	3.5348455E+03	-1.2433202E-03	-6.9394483E-04	2.9877826E-04	7.3078820E-05
391	7.3220404E+03	-2.9812421E-04	-1.6799494E-04	7.3538561E-05	1.8143947E-05
392	1.5571453E+04	-6.5763503E-05	-3.6294888E-05	1.5444178E-05	3.7554984E-06
393	3.4144729E+04	-1.5152583E-05	-8,6075592E-06	3.8213515E-06	9.4970447E-07
304	7 7552073E+04	-2 7567/1/F-06	-1 /002716E-06	6 1570/20E-07	1 4740009E-07
2054	4.00047000.05	2.10014148 00	1.40027100 00	0.10154200 07	1.4140000E 01
395	1.8331/66E+05	-8.5925459E-07	-4.8980789E-07	2.1885493E-07	5.45/0/3/E-08
396					
397					
398	1.9453737E-02	-4.7665861E-09	8.1805294E-09	-3.6249172E-08	-2.6296851E-05
399	3.6141658E-02	1.9195897E-08	-4.2306839E-08	2.1627369E-07	-1.9156671E-04
400	6 71/53538-02	-/ 88/0001E-08	1 23/3567F-07	-/ 10/0585F-07	-5 8/6760/F-0/
401	1 0474010E 01	1 0200420E 07	1.2040001E 07	1 00004515 06	1 0760744E 02
401	1.24/40106-01	1.0300432E-07	-2.90410086-07	1.99004516-00	-1.0/02/446-03
402	2.3178217E-01	-2.0414601E-07	5.9173652E-07	6.7275140E-06	-1.4572199E-03
403	4.3071120E-01	3.8613103E-07	-1.3933250E-06	1.6059381E-04	-1.3152239E-03
404	8.0058681E-01	-7.1410391E-07	1.7536461E-06	1.3171861E-03	-3.3708597E-04
405	1.4887931E+00	1.3136455E-06	3.3901664E-06	4 7746749E-03	1.4319939E-03
406	2 7707233E+00	-1 9267861E-06	3 /710011E-0/	7 5386331E-03	2 3753685E-03
407	2.11012335100	1.3207001E 00	0.05400400 00	0.303000010 00	2.3733003E 03
407	0.1020048E+00	1.4123028E-07	3.0040012E-03	2.1310309E-03	5.002/200E-04
408	9.6361639E+00	-1.1191286E-04	1.3605693E-02	-1.2944336E-03	-1.8194942E-03
409	1.8031447E+01	-2.1949542E-03	1.6976115E-02	-9.8769744E-03	-2.5306567E-03
410	3.3858337E+01	-1.2885923E-02	3.0958817E-03	-2.7485193E-03	-7.2321262E-04
411	6.3875692E+01	-2.9036735E-02	-1.4706197E-02	6.1253089E-03	1.4911026E-03
419	1 21251778-02	-3 21400785-02	-1 87033535-00	8 19568208-02	2 01635005-02
410	1.21201/1E+U2	-0 0E60700E 00	_1 2141606E 00	E 7240004E 00	1 40706265 00
413	2.3200920E+02	-2.2569729E-02	-1.3141606E-02	5.7348291E-03	1.4079636E-03
414	4.4845175E+02	-1.1722481E-02	-6.7283794E-03	2.9373860E-03	7.2227047E-04
415	8.7781809E+02	-4.9597391E-03	-2.7988715E-03	1.2118459E-03	2.9706335E-04
416	1.7450942E+03	-1.8420135E-03	-1.0375926E-03	4.5193033E-04	1.1118511E-04
417	3 53/8/558+03	-6 1075133E-04	-3 3063620F-04	1 46002295-04	3 56906228-05
419	7 2000404E+02	-1 0/17120E-04	-1 00040505-04	4 7000220E 04	1 1000124E_0E
410	7.3220404E+03	-1.941/130E-04	-1.0924950E-04	4.7692364E-05	1.1020134E-05
419	1.5571453E+04	-5.5414419E-05	-3.0380139E-05	1.2843419E-05	3.1128767E-06
420	3.4144729E+04	-1.6218355E-05	-9.2679551E-06	4.1602860E-06	1.0398485E-06
421	7.7552073E+04	-3.6486776E-06	-1.9252975E-06	7.6724542E-07	1.7990722E-07
422	1.8331766E+05	-1.2882697E-06	-7.5080026E-07	3.4612983E-07	8.7631389E-08
423					
494					
424		10	FP		
420		41-	51-		
426		-1 //28301/F+01	-0 00125445-01		
		1.42033146.01	-2.92135446-01		
427		1.42033146.01	-2.9213544E-01		
$427 \\ 428$		1.42033146.01	-2.9213344E-01		
427 428 429	1 94537375-02	6 65193/3E-06	-7.5234628E-05		
427 428 429	1.9453737E-02	6.6519343E-06	-7.5234628E-05		
427 428 429 430	1.9453737E-02 3.6141658E-02	6.6519343E-06 -2.1360454E-05	-7.5234628E-05 -2.6536652E-03		
427 428 429 430 431	1.9453737E-02 3.6141658E-02 6.7145353E-02	6.6519343E-06 -2.1360454E-05 4.6289376E-05	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02		
427 428 429 430 431 432	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02		
427 428 429 430 431 432 433	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 1.2967025E-04	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01		
427 428 429 430 431 432 433 434	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 1.2967025E-04 -1.3368066E-04	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.2013932E-01		
427 428 429 430 431 432 433 434 435	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0055661E-01	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 1.2967025E-04 -1.3368066E-04 4.0938667E-04	-7.5234628E-01 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997398E-01 -2.2013932E-01 -2.9387764E-01		
427 428 429 430 431 432 433 434 435 436	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E-00	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 1.2967025E-04 -1.3368066E-04 4.0938667E-04 3.0219209E-03	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.2013932E-01 -2.9387764E-01		
$\begin{array}{r} 427 \\ 428 \\ 429 \\ 430 \\ 431 \\ 432 \\ 433 \\ 434 \\ 435 \\ 436 \\ 427 \end{array}$	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E+00 2.707328E+00	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 1.3967052E-04 -1.3368066E-04 3.0219209E-03 2.7891472E-00	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.9387764E-01 -3.0617901E-01 -3.0617901E-01		
427 428 429 430 431 432 433 434 435 436 437 428	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E+00 2.7707233E+00 2.7707233E+00	6.6519343E-06 -2.1360454E-05 4.6289376E-05 1.2967025E-04 -1.3368066E-04 4.0938667E-04 3.0219209E-03 3.7821876E-02 4.2007E-04	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.2013932E-01 -3.0617901E-01 -3.0617901E-01 -2.297888E-01		
427 428 429 430 431 432 433 434 435 436 437 438 436	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0056681E-01 1.4887931E+00 2.7707233E+00 5.1625848E+00	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 -1.3368066E-04 4.0938667E-04 3.0219209E-03 3.7821876E-02 1.5394501E-01	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.2013932E-01 -3.0617901E-01 -2.2297888E-01 -7.7968302E-02		
427 428 429 430 431 432 433 434 435 436 437 438 439	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 1.4887931E+00 2.7707233E+00 2.7707233E+00 5.1625848E+00 9.6361639E+00	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 1.2967025E-04 4.0938667E-04 3.0219209E-03 3.7821876E-01 3.0647180E-01	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.2013932E-01 -2.9387764E-01 -3.0617901E-01 -7.7968302E-02 5.1295935E-02		
$\begin{array}{r} 427\\ 428\\ 429\\ 430\\ 431\\ 432\\ 433\\ 434\\ 435\\ 436\\ 437\\ 438\\ 439\\ 440\\ \end{array}$	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0055681E-01 1.4887931E+00 2.7707233E+00 5.1625848E+00 1.8031447E+01	6.6519343E-06 -2.1360454E-05 4.6289376E-05 -6.6350273E-05 1.2967025E-04 -1.3368066E-04 4.0938667E-04 3.0219209E-03 3.7821876E-02 1.5394501E-01 3.0647180E-01 3.4548477E-01	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.2013932E-01 -2.9387764E-01 -3.0617901E-01 -2.2297888E-01 -7.7968302E-02 5.1295935E-02 9.1788477E-02		
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$\begin{array}{r} 427\\ 428\\ 429\\ 430\\ 431\\ 432\\ 433\\ 434\\ 435\\ 436\\ 437\\ 438\\ 439\\ 440\\ 441\\ 442\\ 443\\ 444\\ 445\\ 444\\ 445\\ 445\\ 445\\ 451\\ 452\\ 454\\ 455\\ 456\\ 455\\ 456\\ 455\\ 456\\ 466\\ 46$	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 3.0058681E-01 1.4887931E+00 2.7707233E+00 9.6361639E+00 1.8031447E+01 3.3858337E+01 6.3875692E+01 1.2125177E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5344455E+03 3.5344455E+03 1.9453737E-02 3.6141658E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4887931E+00 2.7707233E+00 5.1625848E+00 9.6361639E+00 1.837692E+01 1.2125177E+02 2.320920E+02 4.4845175E+02 8.37781809E+02 1.7450942E+03 3.5348455E+03 3.5348455E+03	6.6519343E-06 -2.1360454E-05 4.6289376E-05 1.2967025E-04 1.3368066E-04 4.0938667E-04 3.0219209E-03 3.7821876E-02 1.5394501E-01 3.0647180E-01 3.4548477E-01 1.2634752E-01 4.5722954E-02 1.3450450E-02 3.1290776E-03 7.5391295E-04 4.9214287E-05 9.7802298E-09 -4.5904641E-08 1.2937723E-07 -6.6021547E-07 -1.0452365E-06 3.7845584E-06 3.9665322E-05 6.8727947E-04 3.236579E-03 1.0396309E-02 1.6086541E-02 1.0396309E-02 2.1331306E-03 1.0396309E-02 2.1331306E-03 1.0336879E-03 1.336879E-03 1.336879E-03 1.33160E-03 6.6181052E-04 2.1331376E-05 1.7481944E-05	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.9387764E-01 -3.0617901E-01 -2.297888E-01 -7.7968302E-02 5.1295935E-02 9.1788477E-02 3.9475329E-03 9.0396660E-04 2.2220654E-04 3.6367372E-05 1.4522570E-05 -1.1425213E-07 -5.5196843E-06 -5.1249869E-05 -2.2864402E-04 -5.5196843E-06 -5.1249869E-05 -2.28778807E-03 -4.069157E-03 -1.9386644E-03 1.7415482E-03 -2.8778807E-03 -1.9386644E-03 1.7415482E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 3.2160372E-03 1.967944E-04 6.2619880E-04 1.9105941E-04 5.2199366E-06		
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$\begin{array}{r} 427\\ 428\\ 429\\ 430\\ 431\\ 432\\ 433\\ 434\\ 435\\ 436\\ 437\\ 448\\ 443\\ 444\\ 445\\ 444\\ 445\\ 444\\ 445\\ 446\\ 451\\ 451\\ 452\\ 453\\ 454\\ 455\\ 456\\ 457\\ 458\\ 459\\ 460\\ 461\\ 465\\ 466\\ 467\\ 468\\ 466\\ 466\\ 467\\ 468\\ 469\\ 470\\ 471\\ 472\\ 472\\ 472\\ 472\\ 472\\ 472\\ 472\\ 472$	1.9453737E-02 3.6141658E-02 6.7145353E-02 1.2474816E-01 2.3178217E-01 4.3071120E-01 1.4387931E+00 2.7707233E+00 2.7707233E+00 3.6361639E+00 1.83875692E+01 1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03 1.9453737E-02 3.6141658E-02 6.7145352E-02 1.2474818E-01 2.3178217E-01 4.3071120E-01 8.0058681E-01 1.4387931E+00 2.7707235E+00 5.1625848E+00 9.6361639E+00 1.631447E+01 3.3858337E+01 6.3875692E+01 1.2125177E+02 2.3200920E+02 4.4845175E+02 8.7781809E+02 1.7450942E+03 3.5348455E+03	6.6519343E-06 -2.1360454E-05 4.6289376E-05 6.6350273E-06 1.2967025E-04 1.3368066E-04 4.0938667E-04 3.0219209E-03 3.7821876E-02 1.5394501E-01 3.6474180E-01 3.6474180E-01 3.6474180E-01 3.6474782E-01 4.5722954E-02 1.2634752E-01 4.5214287E-05 9.7802298E-09 -4.5904641E-08 1.2634752E-01 4.9214287E-05 9.7802298E-09 -4.5904641E-08 3.7845584E-06 3.7845784E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784584E-06 3.784	-7.5234628E-05 -2.6536652E-03 -1.8069774E-02 -5.9145321E-02 -1.2997399E-01 -2.2013932E-01 -2.2013932E-01 -2.2013932E-01 -2.2297888E-01 -7.7968302E-02 5.1295935E-02 9.1788477E-02 7.2862946E-02 3.7217372E-02 1.3327572E-02 3.7217372E-02 1.3327572E-02 3.9039660E-04 2.220654E-04 3.6367372E-05 -1.4522570E-05 -1.4522570E-05 -2.2864402E-04 4.68490365E-04 -1.5812801E-03 -2.887492E-03 4.0609157E-03 1.7415482E-03 4.261347758E-03 4.261347758E-03 3.2160372E-03 1.5670944E-03 6.2619880E-04 1.9105941E-04 4.0086793E-05 1.2694798E-05 5.2199366E-06		

474	-1.3899400E+01	-2.7004390E-01	
475			
476	1 94537375-02 -7 57107555-06	1 43587298-04	
478	3.6141658E-02 2.4162114E-05	3.7346339E-03	
479	6.7145353E-02 -5.2886361E-05	2.2106892E-02	
480	1.2474818E-01 7.4984490E-05	6.6652471E-02	
481	2.3178217E-01 -1.4619715E-04	1.3906611E-01	
482	4.30/1120E-01 1.5321002E-04 8.0058681E-01 -4.5908422E-04	2.2654866E-01 2.9384540E-01	
484	1.4887931E+00 -3.4599894E-03	3.0112350E-01	
485	2.7707233E+00 -4.0854397E-02	2.1487666E-01	
486	5.1625848E+00 -1.6027303E-01	6.9670258E-02	
487	9.6361639E+00 -3.1187985E-01	-5.4403079E-02	
489	3.3858337E+01 -2.4827600E-01	-7.0373982E-02	
490	6.3875692E+01 -1.2151771E-01	-3.5284216E-02	
491	1.2125177E+02 -4.2830578E-02	-1.2308746E-02	
492	2.3200920E+02 -1.2088313E-02	-3.4969605E-03	
493	4.4845175E+02 -2.6662822E-03 8 7781809E+02 -5 7540121E-04	-7.5896215E-04 -1.6751694F-04	
495	1.7450942E+03 -8.8544591E-05	-2.4524420E-05	
496	3.5348455E+03 -2.3576924E-05	-6.9470986E-06	
497			
498	1 9453737E-02 -1 2101571E-08	2 19079645-07	
500	3.6141658E-02 5.1973800E-08	7.7720385E-06	
501	6.7145353E-02 -1.5341845E-07	6.2702951E-05	
502	1.2474818E-01 2.9575690E-07	2.5768755E-04	
503	2.3178217E-01 -7.7984903E-07	7.3285185E-04	
504	4.30/1120E-01 1.115326/E-06 8.0058681E-01 -4.5192354E-06	2.8778425E-03	
506	1.4887931E+00 -4.6192042E-05	4.0215028E-03	
507	2.7707233E+00 -7.4463276E-04	3.9142810E-03	
508	5.1625848E+00 -3.9866749E-03	1.7314970E-03	
509	9.6361639E+00 -1.0595697E-02 1 8031447E+01 -1 5983972E-02	-1.848/122E-03 -4 2120077E-03	
511	3.3858337E+01 -1.5775294E-02	-4.4706439E-03	
512	6.3875692E+01 -1.0569570E-02	-3.0682566E-03	
513	1.2125177E+02 -5.1013080E-03	-1.4655355E-03	
515	2.3200920E+02 -1.9715140E-03 4 4845175E+02 -5 9357692E-04	-5.7017825E-04 -1.6884944E-04	
516	8.7781809E+02 -1.7454005E-04	-5.0836243E-05	
517	1.7450942E+03 -3.6449349E-05	-1.0060536E-05	
518	3.5348455E+03 -1.2858668E-05	-3.8037142E-06	
519 520			
519 520 521	Calculated energy = -2.7274	376153339403E+04	
519 520 521 522	Calculated energy = -2.7274 Literature energy = -2.7274	376153339403E+04 378906250000E+04	
519 520 521 522 523 524	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75	376153339403E+04 378906250000E+04 E-03	
519 520 521 522 523 524 525	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272	74.37615333940
519 520 521 522 523 524 525 526	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 40	376153339403E+04 378906250000E+04 E-03 b)/lit)) = 1.01E-07 Final energy = -272 Final energy = -272	74.37615333940 74.37652373574
519 520 521 522 523 524 525 526 527	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 39	376153339403E+04 378906250000E+04 E-03 b)/lit)) = 1.01E-07 Final energy = -272 Final energy = -272 Final energy = -272	74.37615333940 74.37652373574 74.36557271042
519 520 521 522 523 524 525 526 527 528 527	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.755 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 39 SCF converged at iteration 39 SCF converged at iteration 30	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final energy = -272 Final energy = -272 Final energy = -272 Final energy = -272	74.37615333940 74.37652373574 74.36557271042 74.37328631207
519 520 521 522 523 524 525 526 527 528 529 530	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 36 SCF converged at iteration 36	376153339403E+04 378906250000E+04 E-03 V/lit)) = 1.01E-07 Final energy = -272 Final energy = -272	74.37615333940 74.37652373574 74.36557271042 74.37328631207 74.37561712200 74.3755675471
519 520 521 522 523 524 525 526 527 528 529 530 531	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 36 SCF converged at iteration 36	376153339403E+04 378906250000E+04 E-03 b/lit)) = 1.01E-07 Final energy = -272 Final energy = -272	74.37615333940 74.37652373574 74.36552721042 74.37328631207 74.37681712200 74.3755675471 74.02325483119
519 520 521 522 523 524 525 526 527 528 529 530 531 532	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 38	376153339403E+04 378906250000E+04 E-03 V/lit)) = 1.01E-07 Final energy = -272 Final energy = -272	74.37615333940 74.37652373574 74.36557271042 74.37328631207 74.37328631207 74.37555675471 74.02325483119 74.37703303956
519 520 521 522 523 524 525 526 527 528 529 530 531 532 532 532	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 38	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.37328631207 74.37328631207 74.37355675471 74.02325483119 74.37703303956 74.37463387263 74.3626262027
519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 534 535	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 38 SCF converged at iteration 40 SCF converged at iteration 40 SCF converged at iteration 40	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final energy = -272	74.37615333940 74.37652373574 74.36557271042 74.37328631207 74.37328631207 74.37555675471 74.02325483119 74.37703303956 74.37463387263 74.36624593227 74.36624593227 74.36624593227
519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 39 SCF converged at iteration 38 SCF converged at iteration 40 SCF converged at iteration 38	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.37328631207 74.37585675471 74.37555675471 74.37555675471 74.37453387263 74.37463387263 74.37463387263 74.36624593227 74.36325682023 74.3675780536
519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 535 536 537	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.756 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 38 SCF converged at iteration 38	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.3768171200 74.37565675471 74.02325483119 74.377573303556 74.3745387263 74.3624593227 74.36624593227 74.36624593227 74.36767506356 74.37705991919
$\begin{array}{c} 519\\ 520\\ 521\\ 522\\ 523\\ 524\\ 526\\ 526\\ 527\\ 528\\ 529\\ 530\\ 531\\ 532\\ 533\\ 534\\ 535\\ 536\\ 537\\ 538\\ 538\\ 538\\ 539\\ \end{array}$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 38 SCF converged at iteration 40 SCF converged at iteration 40	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.375328631207 74.3756575471 74.3755675471 74.3755675471 74.3745387263 74.3463387263 74.36624593227 74.36258652023 74.36624593227 74.37675991919 74.377711582447 74.36256340017
$\begin{array}{c} 519\\ 520\\ 521\\ 522\\ 523\\ 524\\ 525\\ 526\\ 527\\ 528\\ 529\\ 530\\ 531\\ 532\\ 533\\ 534\\ 535\\ 536\\ 537\\ 538\\ 539\\ 540\\ \end{array}$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 38 SCF converged at iteration 40 SCF converged at iteration 40	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.375328631207 74.375681712200 74.3755675471 74.02325483119 74.3770303956 74.37463387263 74.3624553227 74.3624553227 74.3624553227 74.36256536 74.37705991919 74.37711582447 74.36256340017 74.37525627186
$\begin{array}{c} 519\\ 520\\ 521\\ 522\\ 523\\ 524\\ 525\\ 526\\ 527\\ 528\\ 529\\ 530\\ 531\\ 532\\ 533\\ 534\\ 535\\ 536\\ 537\\ 538\\ 539\\ 540\\ 541\\ \end{array}$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.37328631207 74.37681712200 74.37556675471 74.02325483119 74.37703303956 74.37463387263 74.3624593227 74.36325682023 74.3675780536 74.37705991919 74.37711582447 74.35252340017 74.3755627186 74.37554430689
5199 5200 5212 5223 5242 5255 5265 5275 5288 5299 5330 5332 5334 5335 5336 5337 5338 5339 5339 5339 5339 5339 5339 5342 5335 5365 5365 5377 5388 5399 5399 5325 5365 5377 5388 5399 5399 5325 5365 5377 5388 5399 5399 5399 5325 5365 5377 5388 5399 5399 5399 5399 5399 5399 5326 5377 5388 5399 5400 5410 5410 5420 5420 5420 5420 5420 5420 5420 5420 5420 5420 5420 5337 5389 5400 5420 540 5400	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 39 SCF converged at iteration 38 SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 V/lit)) = 1.01E-07 Final energy = -272 Final ener	74.37615333940 74.37652373574 74.36557271042 74.37328631207 74.37328631207 74.37555675471 74.02325483119 74.37703303956 74.3745387263 74.3624593227 74.36325683223 74.3675780536 74.3770591919 74.37711582447 74.37525627186 74.37525627186 74.37525819958 74.37525819958
$\begin{array}{c} 519\\ 520\\ 521\\ 522\\ 523\\ 524\\ 525\\ 526\\ 527\\ 528\\ 529\\ 530\\ 531\\ 532\\ 533\\ 534\\ 535\\ 536\\ 537\\ 538\\ 536\\ 537\\ 538\\ 540\\ 541\\ 542\\ 543\\ 544\\ 544\\ 544\\ 544\\ 544\\ 544\\ 544$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.37652373574 74.36557271042 74.3755675471 74.37555675471 74.37653675471 74.37453387263 74.37463387263 74.36624593227 74.3625682023 74.36624593227 74.3625682023 74.37675780536 74.37705991919 74.3775780536 74.37525627186 74.375256340017 74.37525619958 74.3752819958 74.375618439044 74.375618439044
$\begin{array}{c} 5199\\ 5200\\ 521\\ 522\\ 523\\ 524\\ 525\\ 526\\ 527\\ 528\\ 539\\ 530\\ 531\\ 532\\ 535\\ 535\\ 535\\ 535\\ 535\\ 536\\ 539\\ 539\\ 540\\ 541\\ 542\\ 543\\ 545\\ \end{array}$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.37657271042 74.37585675471 74.37585675471 74.37585675471 74.37453387263 74.37463387263 74.36624593227 74.36325682023 74.3625682023 74.37675780536 74.37705991919 74.37705991919 74.377525627186 74.37525627186 74.375256340017 74.375256430689 74.37525419958 74.37618439044 74.37569386304 4.377 115 824 5 -27274.377 115 824 5
$\begin{array}{c} 5199\\ 5200\\ 5212\\ 5223\\ 5224\\ 5255\\ 5266\\ 5277\\ 5288\\ 5299\\ 5302\\ 5331\\ 5322\\ 5333\\ 5342\\ 5355\\ 5366\\ 5377\\ 5388\\ 5399\\ 5411\\ 5422\\ 5433\\ 5442\\ 5455\\ 5465\\ 5456\\$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 40 SCF converged 40 SCF converged 40 SCF converged 40 SCF converged 40 S	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.376557271042 74.376567271042 74.3756675471 74.02325483119 74.37453675471 74.3746387263 74.36624593227 74.36624593227 74.3662780536 74.37711582447 74.37675991919 74.37711582447 74.3652540017 74.35525627186 74.375543069 74.37554319588 74.375618439044 74.37569386304 4.377 115 824 5 1.0000000
5199 5201 5212 523 5245 5255 5255 5255 5266 5277 5288 5330 5332 5334 5335 5336 5335 5336 5337 5338 5339 5440 5442 5445 5456 5566 5566 5566 5566 5566 5566 5566 5566 5566	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 40 SCF conve	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.3753667112200 74.3755675471 74.02325483119 74.37453675471 74.37463387263 74.36624593227 74.36624593227 74.36325682023 74.37675991919 74.377711582447 74.36526340017 74.3755427186 74.3755427186 74.3755439683 4.3775593968 4.377115 824 5 1.0000000 74.37624394280 74.37654394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.3765958 74.3765958 74.3765958 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.5777 75.57777 75.5777 75.57777 75.577777 75.5777777 75.5
$\begin{array}{c} 5199\\ 5201\\ 5212\\ 523\\ 525\\ 525\\ 525\\ 525\\ 526\\ 529\\ 530\\ 5332\\ 5332\\ 5335\\ 5336\\ 5335\\ 5336\\ 5336\\ 5336\\ 5342\\ 5445\\ 5445\\ 5446\\ 5447\\ 548\\ 549\\ \end{array}$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.37536675471 74.37555675471 74.37555675471 74.3745387263 74.3746387263 74.36624593227 74.36624593227 74.36325682023 74.3765780536 74.3705991919 74.37711582447 74.36526340017 74.3755430689 74.3755430689 74.3755430689 74.3755430689 74.37659386304 4.377 115 824 5 1.000000 74.37661479764 74.37661479764 74.37661479764 74.37661479764 74.376624394280 74.37661479764 74.376624394280 74.37661479764 74.376624394280 74.37661479764 74.376624394280 74.37661479764 74.376624394280 74.37661479764 74.37661479764 74.3760584840
$\begin{array}{c} 5190\\ 5201\\ 5212\\ 5233\\ 5242\\ 5245\\ 5265\\ 5285\\ 5286\\ 5299\\ 5302\\ 5312\\ 5332\\ 5335\\ 5355\\ 5355\\ 5356\\ 5377\\ 5389\\ 5402\\ 5412\\ 5433\\ 5444\\ 5455\\ 5466\\ 5477\\ 5488\\ 5466\\ 5477\\ 5488\\ 5500\\$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 37 SCF converged at iteration 38 SCF converged at iteration 40 SCF conve	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.3758675741 74.3755675471 74.3755675471 74.37546387263 74.37463387263 74.3624583227 74.3624583227 74.3624583227 74.3625630017 74.3705991919 74.37711582447 74.36526340017 74.37552627186 74.375543430649 74.375543430649 74.37559386304 4.377 115 824 5 1.000000 74.37624394280 74.37643494280 74.376648440 74.37660684840 74.37710938528
$\begin{array}{c} 5190\\ 5201\\ 5212\\ 5233\\ 5242\\ 5255\\ 5266\\ 527\\ 528\\ 529\\ 5302\\ 531\\ 5322\\ 5335\\ 5342\\ 5355\\ 537\\ 538\\ 540\\ 5412\\ 5433\\ 5444\\ 5445\\ 5445\\ 5446\\ 5447\\ 5488\\ 549\\ 549\\ 5500\\ 5510\\ 5500\\ 5510\\ 5500\\ 5510\\ 5500\\ 5510\\ 5500\\ 55$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36552721042 74.37328631207 74.37681712200 74.37555675471 74.02325483119 74.37703303956 74.37463387263 74.3765580536 74.37705991919 74.37705780536 74.3770552819958 74.375525819958 74.3755430044 74.37555430044 74.3755439044 74.37661439044 74.37661439044 74.37661479764 74.37661479764 74.3770938528 74.3770990601
519 5201 5222 523 5242 5255 5265 5265 5275 5282 5299 5311 5322 5334 5335 5343 5335 5365 5375 5388 5399 5411 5442 5443 5445 5445 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5445 5446 5477 5488 5490 5571 5572	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.376557271042 74.37655675471 74.37658675471 74.37658675471 74.37453387263 74.36624593227 74.36325682023 74.3625682023 74.3625682023 74.37675780536 74.37705991919 74.377525627186 74.37525627186 74.37525627186 74.375256340017 74.375256430689 74.37525619958 74.37618439044 74.37569386304 4.377 115 824 5 1.000000 74.37624394280 74.376604840 74.37710938528 74.37710938528 74.37712130963 74.37712130963
$\begin{array}{r} 5190\\ 5201\\ 5222\\ 5233\\ 524\\ 525\\ 526\\ 527\\ 528\\ 529\\ 531\\ 532\\ 533\\ 533\\ 533\\ 533\\ 533\\ 533\\ 533$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.3755675271042 74.376512200 74.37651200 74.3765875471 74.37453387263 74.36624593227 74.36325682023 74.3625682023 74.3765780536 74.37705991919 74.3775563267186 74.377558439689 74.37525627186 74.37556343044 74.37525634958 74.37618439044 74.37569386304 74.37624334280 74.37624334280 74.37664384280 74.37664384280 74.37664384280 74.37664384280 74.3771138528 74.37712130963 74.37712130963 74.37716226352 74.377142678
$\begin{array}{r} 5199\\ 5201\\ 5222\\ 5232\\ 5242\\ 5255\\ 5266\\ 5277\\ 5288\\ 5299\\ 5301\\ 5312\\ 5332\\ 5334\\ 5355\\ 5366\\ 5377\\ 5388\\ 5401\\ 5412\\ 5466\\ 5477\\ 5489\\ 5546\\ 5477\\ 5489\\ 5501\\ 5552\\ 5553\\ 5552\\ 5553\\ 5552\\ 5553\\ 5552\\$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 40 SCF conve	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.376567271042 74.3765675471 74.02325483119 74.37703303956 74.3624593227 74.3624593227 74.3625680203 74.3767580536 74.3775591919 74.3775569360 74.37556430017 74.3755643004 74.37556430989 74.3755643094 74.37556386304 4.377 115 824 5 1.000000 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37709990601 74.37711230963 74.37716226352 74.3771672333
$\begin{array}{r} 5199\\ 5201\\ 5222\\ 5232\\ 5242\\ 5255\\ 5265\\ 5277\\ 5288\\ 5299\\ 5301\\ 5332\\ 5334\\ 5355\\ 5364\\ 5375\\ 5388\\ 5395\\ 5364\\ 5455\\ 5466\\ 5477\\ 5488\\ 5499\\ 5501\\ 5546\\ 5465\\$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 40 SCF conve	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.3756575471 74.3755575471 74.3763575471 74.3745387263 74.36624593227 74.3624593227 74.36325682023 74.37659580536 74.37755991919 74.377711582447 74.36526340017 74.37555427186 74.3755439683 74.375543968 74.375543968 74.37659386304 4.377 115 824 5 1.0000000 74.37624394280 74.37624394280 74.37710938528 74.3771938528 74.3771920651 74.3771422678 74.377095333 74.377095333 74.377095337
519 5201 5222 5232 5242 5255 5265 5275 5288 5290 5311 5332 5332 5334 5335 5336 5337 5388 5390 5411 5423 5443 5443 5443 5443 5444 5455 5465 5477 5488 5490 5412 5423 5444 5455 5465 5477 5488 5490 5452 5465 5477 5488 5490 5555 5556 5557 5555	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 38 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.375687112200 74.3756575471 74.02325483119 74.3745387263 74.3642583227 74.3624583227 74.36325682023 74.3765780536 74.3705991919 74.37711582447 74.36526340017 74.37552627186 74.3755430689 74.3755430689 74.3755430958 74.37654394280 74.37661479764 74.37661479764 74.37710938528 74.37719308528 74.37719263537 74.3771742678 74.37717330824 74.37717330824 74.37717330824 74.37707300000
$\begin{array}{r} 5199\\ 5201\\ 5222\\ 5233\\ 524\\ 525\\ 526\\ 529\\ 529\\ 529\\ 529\\ 530\\ 531\\ 533\\ 534\\ 533\\ 534\\ 533\\ 534\\ 533\\ 534\\ 545\\ 536\\ 542\\ 542\\ 544\\ 545\\ 554\\ 556\\ 557\\ 558\\ 556\\ 557\\ 558\\ 556\\ 557\\ 558\\ 556\\ 557\\ 558\\ 556\\ 557\\ 558\\ 556\\ 557\\ 558\\ 556\\ 557\\ 558\\ 556\\ 557\\ 558\\ 556\\ 556\\ 557\\ 558\\ 556\\ 556\\ 556\\ 556\\ 556\\ 556\\ 556$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.3758675741 74.3755675471 74.3755675471 74.3746387263 74.3746387263 74.3624583227 74.3624583227 74.36256380307 74.3705780536 74.37705991919 74.37711582447 74.37525819958 74.37552627186 74.37554330649 74.37559386304 4.377 115 824 5 1.0000000 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.37624394280 74.377624394280 74.37714938528 74.37719938528 74.37714226352 74.377142268 74.37717330824 74.37717330824 74.37710224991 74.37710224991 74.377147200
$\begin{array}{r} 519\\ 520\\ 522\\ 522\\ 522\\ 522\\ 522\\ 522\\ 522$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 30 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 t)/lit)) = 1.01E-07 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.376587271042 74.37658675471 74.3763872200 74.3763387263 74.36624593227 74.36325682023 74.3625682023 74.3625682023 74.3765780536 74.37705991919 74.3775562340017 74.37525627186 74.37556430689 74.37556430689 74.37556430689 74.37556386304 4.377 115 824 5 1.000000 74.37624394280 74.37660684840 74.37710938528 74.3771622352 74.377171230963 74.3771622352 74.3771622352 74.37717422678 74.37717422740 74.3770601249
$\begin{array}{r} 5199\\ 5201\\ 5222\\ 5233\\ 524\\ 525\\ 5266\\ 527\\ 5288\\ 530\\ 531\\ 532\\ 5333\\ 534\\ 535\\ 533\\ 534\\ 535\\ 536\\ 537\\ 538\\ 545\\ 545\\ 545\\ 545\\ 545\\ 545\\ 545\\ 554\\ 555\\ 555\\ 555\\ 555\\ 555\\ 555\\ 555\\ 555\\ 556\\ 555\\ 556\\ 555\\ 556\\ 555\\ 556\\ 555\\ 556\\ 555\\ 556\\ 556\\ 555\\ 556\\ 56$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 40 SCF conver	376153339403E+04 378906250000E+04 E-03 Yinal energy = -272 Final energy = -272	74.37615333940 74.37652373574 74.36557271042 74.376557271042 74.3765875271042 74.3765875271042 74.376387220 74.3763387263 74.3763387263 74.3763387263 74.3765780536 74.37705991919 74.37705991919 74.377059302 74.37625627186 74.377558439089 74.37556430689 74.37556430689 74.37556430689 74.37556386304 74.37556386304 74.377569386304 74.37624334280 74.37664384280 74.37664384280 74.3771622333 74.37709665337 74.3771622333 74.37709655337 74.37709624991 74.3771427240 74.3771427240 74.3771971213
519 520 5221 5223 5244 5255 5266 5277 5288 5290 5313 5332 5333 5344 5355 5366 5377 5388 5390 5421 5452 54545 5452 54545 5452 54545 5452 5455 5546 5577 5522 5543 5452 5455 5546 5577 5522 5552 5556 5552 5556 5552 5556 5557 5556 5557 5558 5556 5557 5558 5556 5557 5566 5578 5556 5578 5556 5578 5569 5562 5578 5569 5562 5578 5569 5562 5578 5569 5562 5578 5569 5562 5578 5569 5562 5578 5569 5562 5578 5569 5562 5578 5569 5562 5578 5569 5578 5578 5569 5578 5578 5578 5578 5578 5578 5578 5579 5578 5579 5578 5579 5578 5579 5579 5578 5579 5579 5579 5578 5579 5579 5579 5579 5578 5579 557	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.75 Relative error (abs((cal - li SCF converged at iteration 38 SCF converged at iteration 40 SCF	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.36557271042 74.376557271042 74.3763575741 74.02325483119 74.37703303956 74.3763387263 74.36624593227 74.3624593227 74.36325682023 74.367580536 74.3775991919 74.3775595627186 74.37556430017 74.35525627186 74.37556386304 4.377 115 824 5 1.000000 74.37624394280 74.3766484904 74.37660684840 74.37716283828 74.3771627333 74.3771672333 74.37717427240 74.37769601249 74.37769601249 74.37769601249 74.3770963789 74.3770963789 74.3771427240 74.37769601249 74.3771637889 74.3771637889 74.37763789 75.3776578 75.37776578 75.3776578 75.37776578 75.3776578 75.37776578 75.37776578 75.3776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.37776578 75.377777777777777777777777777777777777
$\begin{array}{r} 5199\\ 5201\\ 5222\\ 5232\\ 5242\\ 5255\\ 5265\\ 5277\\ 5288\\ 5299\\ 5301\\ 5312\\ 5332\\ 5334\\ 5355\\ 5364\\ 5377\\ 5388\\ 5401\\ 5412\\ 5433\\ 5445\\ 5465\\ 5477\\ 5489\\ 5501\\ 5552\\ 5555\\ 5558\\ 5556\\ 5557\\ 5558\\ 5559\\ 5558\\ 5556\\ 5558\\ 5559\\ 5558\\ 5558\\ 5558\\ 5559\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5558\\ 5568\\ 5558\\$	Calculated energy = -2.7274 Literature energy = -2.7274 Difference (cal - lit) = 2.757 Relative error (abs((cal - li SCF converged at iteration 36 SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 30 SCF converged at iteration 40 SCF conve	376153339403E+04 378906250000E+04 E-03 Final energy = -272 Final ene	74.37615333940 74.37652373574 74.375657271042 74.3756575471 74.37555675471 74.3763367263 74.36624593227 74.36624593227 74.3625680203 74.3767580536 74.3775591919 74.37775591919 74.377556938630 74.37556430689 74.37556430689 74.37556386304 4.377 115 824 5 1.0000000 74.37624394280 74.3766434948 74.3766434948 74.3776990611 74.37716226352 74.3771672333 74.3771672333 74.3770924991 74.37717442788 74.3771672333 74.37709224991 74.3771637889 74.3771623852 74.3771637889 74.3771637889 74.3771637889 74.3771637889 74.3771637889 74.37716637889 74.37716637889 74.37716637889 74.37716637889 74.37716637889 74.3771639343

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566	SCF	converged	at	iteration	40	Final	energy	=	-27274.37697998060
567	SCF	converged	at	iteration	40	Final	energy	=	-27274.37719820330
568	SCF	converged	at	iteration	40	Final	energy	=	-27274.37720555374
569	SCF	converged	at	iteration	40	Final	energy	=	-27274.37721015110
570	SCF	converged	at	iteration	40	Final	energy	=	-27274.37721989711
571	SCF	converged	at	iteration	40	Final	energy	=	-27274.37723141619
572	SCF	converged	at	iteration	40	Final	energy	=	-27274.37724506508
573	SCF	converged	at	iteration	40	Final	energy	=	-27274.37727356602
574	SCF	converged	at	iteration	40	Final	energy	=	-27274.37726115421
575	SCF	converged	at	iteration	40	Final	energy	=	-27274.37679573947
576	SCF	converged	at	iteration	40	Final	energy	=	-27274.37729431578
577	SCF	converged	at	iteration	40	Final	energy	=	-27274.37731317497
578	SCF	converged	at -+	iteration	40	Final	energy	Ξ.	-2/2/4.3//32184126
520	SCF	converged	at at	iteration	40	Final	energy	2	-27274.37734102629
591	SCF	converged	at 0+	iteration	40	Final	energy	Ξ.	-27274.37737423937
582	SCF	converged	at	iteration	40	Final	energy	2	-27274 37747058523
583	SCF	converged	at	iteration	41	Final	energy	=	-27274_37143110862
584	SCF	converged	at	iteration	41	Final	energy	=	-27274.37751839181
585	SCF	converged	at	iteration	41	Final	energy	=	-27274.37753025332
586	SCF	converged	at	iteration	40	Final	energy	=	-27274.37668602075
587	SCF	converged	at	iteration	41	Final	energy	=	-27274.37739254861
588	SCF	converged	at	iteration	41	Final	energy	=	-27274.37729343396
589	SCF	converged	at	iteration	41	Final	energy	=	-27274.37753046981
590	SCF	converged	at	iteration	41	Final	energy	=	-27274.37738289865
591	SCF	converged	at	iteration	41	Final	energy	=	-27274.37745108623
592	SCF	converged	at	iteration	41	Final	energy	=	-27274.37745035628
593	SCF	converged	at	iteration	41	Final	energy	=	-27274.37752038428
594	SCF	converged	at	iteration	41	Final	energy	=	-2/2/4.3//4/841063
506	SCF	converged	at at	iteration	41	Final	energy	2	-27274.37753190090
507	SCF	converged	at at	iteration	41	Final	energy	2	-27274.37753338037
598	SCF	converged	at	iteration	41	Final	energy	2	-27274 37739192332
599	SCF	converged	at	iteration	41	Final	energy	2	-27274 37753340209
600	SCF	converged	at	iteration	41	Final	energy	=	-27274.37753764559
601	SCF	converged	at	iteration	41	Final	energy	=	-27274.37753647355
602	SCF	converged	at	iteration	41	Final	energy	=	-27274.37743857712
603	SCF	converged	at	iteration	41	Final	energy	=	-27274.37753417706
604	SCF	converged	at	iteration	41	Final	energy	=	-27274.37746150104
605	SCF	converged	at	iteration	41	Final	energy	=	-27274.37753562298
606	SCF	converged	at	iteration	41	Final	energy	=	-27274.37727249676
607	SCF	converged	at	iteration	41	Final	energy	=	-27274.37753843775
608	SCF	converged	at	iteration	41	Final	energy	=	-27274.37743420742
609	SCF	converged	at	iteration	41	Final	energy	=	-27274.37744247752
610	SCF	converged	-a+t	itoration	41	Final	000000000	=	-27274 37753800378
011	aan		a	iteration			energy		07074 07750444060
611	SCF	converged	at	iteration	41	Final	energy	=	-27274.37752144962
611 612 613	SCF SCF	converged interm	at at at	iteration iteration	41 41 0.0	Final Final	energy energy 000 8	=	-27274.37752144962 -27274.37753749272 -27274.377 538 437 7
611 612 613 614	SCF SCF	converged converged interm	at at rho 7416	iteration iteration o nf F del 5 1.0	41 41 0.0	Final Final 0010000	energy energy 000 8	= 36)254	-27274.37752144962 -27274.37753749272 -27274.377 538 437 7 4277 1.0623435
611 612 613 614 615	SCF SCF ::: SCF	converged converged interm > 1.6627 converged	at at rho 7416 at	iteration iteration o nf F del 6 1.0 iteration	41 41 0.0 002: 41	Final Final 0010000 1141 Final	energy energy 000 8 1.0 energy	= 36)254	-27274.37752144962 -27274.37753749272 -27274.377 538 437 7 4277 1.0623435 -27274.37753764903
611 612 613 614 615 616	SCF SCF ::: SCF SCF	converged interm > 1.6627 converged converged	at at rho 7410 at at	iteration iteration o nf F del 6 1.0 iteration iteration	41 41 0.0 002: 41 41	Final Final 0010000 1141 Final Final	energy energy 000 8 1.0 energy energy	= 36)254 = =	-27274.37752144962 -27274.37753749272 -27274.37753749272 -27274.377538 437 7 1.0623435 -27274.37753764903 -27274.37753839733
611 612 613 614 615 616 617	SCF SCF SCF SCF SCF SCF	converged interm > 1.6627 converged converged converged	at at rho 7410 at at at	iteration iteration onf F del 6 1.0 iteration iteration iteration	41 41 0.0 002: 41 41 41	Final Final 0010000 1141 Final Final Final	energy energy 000 8 1.0 energy energy energy	= 36 0254 = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753864903 -27274.37753839733 -27274.37753831774
611 612 613 614 615 616 617 618	SCF SCF SCF SCF SCF SCF SCF	converged interm > 1.662 converged converged converged converged	at at rho 7410 at at at at	iteration iteration onf F del 5 1.0 iteration iteration iteration iteration	41 41 0.0 002: 41 41 41 41 41	Final Final 0010000 1141 Final Final Final Final	energy energy 200 8 1.0 energy energy energy energy	= 36)254 = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753764903 -27274.37753839733 -27274.3775381774 -27274.3775381774
611 612 613 614 615 616 617 618 619	SCF SCF SCF SCF SCF SCF SCF SCF	converged interm > 1.6627 converged converged converged converged converged	at at rho 7410 at at at at at	iteration iteration o nf F del 5 1.0 iteration iteration iteration iteration	41 41 0.0 202: 41 41 41 41 41 41	Final Final 0010000 1141 Final Final Final Final	energy energy 200 8 1.0 energy energy energy energy energy energy	= 36 0254 = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753764903 -27274.37753839733 -27274.37753881774 -27274.37753986531 -27274.37753966563
$\begin{array}{c} 611 \\ 612 \\ 613 \\ 614 \\ 615 \\ 616 \\ 617 \\ 618 \\ 619 \\ 620 \\ 021 \end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF	converged interm > 1.6627 converged converged converged converged converged	at at rho 7410 at at at at at at	iteration iteration on fF del 5 1.0 iteration iteration iteration iteration iteration	41 41 0.0 002: 41 41 41 41 41 41 41	Final Final 0010000 1141 Final Final Final Final Final	energy energy 200 8 1.0 energy energy energy energy energy energy	= 36)254 = = = =	-27274.37752144962 -27274.37753749272 -27274.377538.437 7 4277 1.0623435 -27274.37753864903 -27274.37753881774 -27274.37753881774 -27274.37753908531 -27274.37753908531 -27274.37753906563 -27274.37753906563
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 620\\ \end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.662 converged converged converged converged converged converged converged</pre>	at at rho 7410 at at at at at at	iteration iteration on f F del 5 1.0 iteration iteration iteration iteration iteration iteration	41 41 0.0 22 41 41 41 41 41 41 41 41 41	Final Final 0010000 1141 Final Final Final Final Final	energy energy 200 8 1.0 energy energy energy energy energy energy energy energy	= 36)254 = = = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.3775383973 -27274.37753839733 -27274.377538908531 -27274.37753906563 -27274.37753966563 -27274.3775400643 -27274.37754022998
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 622\\ 622\end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.662 converged converged converged converged converged converged converged</pre>	at at rho 7410 at at at at at at	iteration iteration on f F del 5 1.0 iteration iteration iteration iteration iteration iteration iteration iteration	41 41 0.()02: 41 41 41 41 41 41 41 41 41 41	Final Final 0010000 1141 Final Final Final Final Final Final	energy energy 2000 8 1.0 energy energy energy energy energy energy energy energy	= 36)254 = = = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753839733 -27274.37753839733 -27274.37753908531 -27274.37753906563 -27274.37754040643 -27274.37754022898 -27274.37754022898 -27274.37754054313 27274.3775405965
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.662T converged converged converged converged converged converged converged converged converged converged</pre>	at at rho 7410 at at at at at at	iteration iteration on f F del f 1.0 iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration	41 41 0.0 02: 41 41 41 41 41 41 41 41 41 41 41	Final Final 0010000 1141 Final Final Final Final Final Final Final Final	energy energy 2000 8 1.0 energy energy energy energy energy energy energy energy energy energy energy	= 36)254 = = = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753839733 -27274.37753839733 -27274.37753861774 -27274.37753966563 -27274.37754040643 -27274.37754040643 -27274.37754045865 -27274.37754015865 -27274.37754015865 -27274.37754015865
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged interm > 1.662; converged converged converged converged converged converged converged converged converged converged converged</pre>	at at rho 7410 at at at at at at at	iteration iteration on f F del iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration	41 41 0.0 02: 41 41 41 41 41 41 41 41 41 41 41 41 41	Final Final 0010000 1141 Final Final Final Final Final Final Final Final Final	energy energy energy energy energy energy energy energy energy energy energy energy energy	= 36)254 = = = = = = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.3775384903 -27274.37753839733 -27274.37753908531 -27274.37753966563 -27274.37754040643 -27274.37754022898 -27274.37754022898 -27274.37754053413 -27274.37754018665 -27274.37754018665 -27274.3775401662
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.662; converged converged converged converged converged converged converged converged converged converged</pre>	at at rho 7410 at at at at at at at	iteration iteration on f F del iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration iteration	$\begin{array}{c} 41 \\ 41 \\ 0.02: \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 4$	Final Final 0010000 1141 Final Final Final Final Final Final Final Final Final	energy energy 200 8 1.0 energy energy energy energy energy energy energy energy energy energy energy	= 36)254 = = = = = = = = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.377538039733 -27274.37753803733 -27274.37753908531 -27274.37753966563 -27274.3775400643 -27274.37754022898 -27274.3775402898 -27274.3775402808 -27274.3775402808 -27274.3775402808 -27274.3775402808 -27274.3775402808 -27274.37754028685 -27274.37754101662 -27274.37754101662 -27274.3775402813
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ \end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.662 converged converged converged converged converged converged converged converged converged converged converged converged converged</pre>	at at rh(7410 at at at at at at at at	iteration iteration on f F del 5 1.0 iteration	$\begin{array}{c} 41 \\ 41 \\ 0.022 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ $	Final Final 0010000 1141 Final Final Final Final Final Final Final Final Final Final Final Final	energy energy energy energy energy energy energy energy energy energy energy energy energy energy energy energy energy energy	= 36 2254 = = = = = = = = = = = = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753839733 -27274.37753839733 -27274.37753908531 -27274.37753966563 -27274.37754040643 -27274.37754040643 -27274.37754015865 -27274.377551040 -27274.37754101662 -27274.37754101662 -27274.37754084213 -27274.3775408969
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ \end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.662 converged converged converged converged converged converged converged converged converged converged converged converged converged converged converged converged</pre>	at at rh() at at at at at at at at at at	iteration iteration on f F del 5 1.0 iteration	$\begin{array}{c} 41 \\ 41 \\ 0.022 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ $	Final Final 0010000 1141 Final Final Final Final Final Final Final Final Final Final Final Final Final Final	energy energy 200 8 1.0 energy energy energy energy energy energy energy energy energy energy energy energy energy energy energy energy energy	= 36 2254 = = = = = = = = = = = = = =	-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753839733 -27274.37753839733 -27274.37753805531 -27274.37753906563 -27274.37754040643 -27274.37754040643 -27274.37754040643 -27274.37754015865 -27274.37754015865 -27274.3775401662 -27274.3775401662 -27274.37754004213 -27274.37754004213 -27274.37754004751
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ \end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.662; converged converged converged converged converged converged converged converged converged converged converged converged converged converged converged converged</pre>	at	iteration iteration of f f del for a second iteration	$\begin{array}{c} 41 \\ 41 \\ 0.0 \\ 02: \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 4$	Final Final 0010000 1141 Final Final Final Final Final Final Final Final Final Final Final Final Final	energy energy 200 8 1.0 energy	= 36)254 = = = = = = = = = = = = = = =	-27274.3775214962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.37753839733 -27274.3775383174 -27274.37753908531 -27274.3775396563 -27274.37754040643 -27274.37754040643 -27274.37754022898 -27274.37754015865 -27274.37754015865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.377540168213 -27274.377540164213 -27274.377540104751 -27274.377531040
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 630\\ \end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	converged interm > 1.6627 converged	at a	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 41 \\ 41 \\ 0.0 \\ 022 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ $	Final Final 0010000 1141 Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final	energy energy 200 8 1.0 energy		-27274.37752144962 -27274.37753749272 -27274.377538437 4277 1.0623435 -27274.37753864903 -27274.37753839733 -27274.37753808531 -27274.37753906563 -27274.37753966563 -27274.37754022898 -27274.37754022898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402865 -27274.37754046213 -27274.37753806969 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 630\\ 631\\ \end{array}$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	converged interm > 1.6627 converged	at at at a at a at a at a at a at a at	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 41\\ 41\\ 0.0\\ 02:\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final O010000 1141 Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final	energy energy 200 8 1.0 energy		-27274.37752144962 -27274.37753749272 -27274.377538 437 7 4277 1.0623435 -27274.37753864903 -27274.37753805733 -27274.37753908531 -27274.37753906563 -27274.37754022898 -27274.3775402898 -27274.37754015865 -27274.37754015865 -27274.37754101662 -27274.37754101662 -27274.37754084213 -27274.37754084213 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 630\\ 631\\ 632\\ 632\\ 632\\ 632\\ 632\\ 632\\ 632\\ 632$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged</pre>	att no. Att att att att att att att att att att	iteration iteration on f F del 5 1.1 iteration	$\begin{array}{c} 41\\ 41\\ 0.0\\ 22\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final O10000 1141 Final Final Final Final Final Final Final Final Final Final Final Final Final Final	energy energy 200 8 1.0.0 energy		-27274.37752144962 -27274.37753749272 -27274.37753749272 -27274.3775384377 4277 1.0623435 -27274.37753839733 -27274.37753839733 -27274.37753908531 -27274.37753906563 -27274.37754040643 -27274.377540422898 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.3775401662 -27274.3775401662 -27274.37754004213 -27274.37754101662 -27274.37754104751 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.377541169751 -27274.37754116962 -27274.377541169751 -27274.37754116962 -27274.377541169751 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.37754179706 -27274.3775417754179706 -27274.37754179706 -27274.37754179706 -27274.375
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 630\\ 631\\ 632\\ 633\\ 633\\ 633\\ 633\\ 633\\ 633\\ 633$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	converged interm > 1.662 converged c	att no. Att a att att att att att att att att at	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 41\\ 41\\ 0.0\\ 22\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final Final	energy energy 000 8 1.0 energy		-27274.37753144962 -27274.37753749272 -27274.377538437 4277 1.0623435 -27274.37753839733 -27274.37753839733 -27274.37753908531 -27274.3775396563 -27274.3775400643 -27274.3775400643 -27274.377540643 -27274.3775401662 -27274.3775401662 -27274.3775410462 -27274.37754104751 -27274.37754104751 -27274.37754116962 -27274.37754116962 -27274.37754118718 -27274.37754138718 -27274.3775418718 -27274.3775418718 -27274.37754175418718 -27274.3775418718 -27274.3775418718 -
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 630\\ 631\\ 632\\ 633\\ 634\\ 634\\ 632\\ 633\\ 634\\ 634\\ 634\\ 635\\ 635\\ 635\\ 635\\ 635\\ 635\\ 635\\ 635$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged</pre>	att	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 41\\ 41\\ 0.0\\ 22\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final	energy energy 000 8 1.0.0 energy		-27274.37752144962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.377538437 -27274.37753839733 -27274.377538381774 -27274.37753908531 -27274.37753966563 -27274.37754022898 -27274.37754022898 -27274.3775402898 -27274.37754016865 -27274.37754101662 -27274.37754101662 -27274.37754084213 -27274.37754084213 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.3775410875 -27274.37754116962 -27274.37754138718 -27274.37754138718 -27274.37754335791
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 630\\ 631\\ 632\\ 633\\ 634\\ 635\\ 635\\ 634\\ 635\\ 635\\ 634\\ 635\\ 635\\ 635\\ 635\\ 635\\ 635\\ 635\\ 635$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	converged interm > 1.662 converged	att no value a a a a a a a a a a a a a a a a a a a	iteration iteration on f F del 5 1.0 iteration	$\begin{array}{c} 41\\ 41\\ 0.02\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final	energy energy 200 8 1.0.0 energy		-27274.37752144962 -27274.37753749272 -27274.3775384957 -27274.377538497 -27274.3775384973 -27274.37753839733 -27274.37753908531 -27274.37753908531 -27274.37754040643 -27274.3775402898 -27274.3775402898 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.3775401662 -27274.37754101662 -27274.377541046213 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754108969 -27274.37754138718 -27274.37754138718 -27274.37754138718 -27274.37754138718 -27274.37754138718 -27274.37754138719 -27274.37754138719 -27274.37754042695 -27274.37754042695
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 630\\ 631\\ 632\\ 633\\ 634\\ 635\\ 636\\ 636\\ 636\\ 636\\ 636\\ 636\\ 636$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged c</pre>	at athomas at a state at at a state at a state at a state at at a state at at a state at at at a state at at at at a state at	iteration iteration of f f del f 1.(iteration	$\begin{array}{c} 41\\ 41\\ 0.02\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final	energy energy 000 8 1.0 energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.377538435 -27274.37753839733 -27274.37753839733 -27274.37753908531 -27274.37753906563 -27274.37754040643 -27274.37754040643 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.3775401662 -27274.3775401662 -27274.3775401662 -27274.37754106963 -27274.3775410696 -27274.3775410962 -27274.37754108751 -27274.3775410896 -27274.37754108751 -27274.37754108751 -27274.37754248896 -27274.3775424896 -27274.3775424895 -27274.3775424895 -27274.3775424895 -27274.377542695 -27274.377540775402695 -27274.3775402695 -27274.3775402695 -27274.377540
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 619\\ 620\\ 620\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 630\\ 633\\ 634\\ 635\\ 636\\ 637\\ 638\\ 834\\ 635\\ 636\\ 637\\ 638\\ 834\\ 635\\ 636\\ 637\\ 638\\ 838\\ 638\\ 638\\ 638\\ 638\\ 638\\ 638$	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged converged interm > 1.6627 converged conve</pre>	att no. 410 att att att att att att att att att at	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 41\\ 41\\ 0.02\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.37753839733 -27274.37753839733 -27274.37753906531 -27274.37753966563 -27274.37754002898 -27274.37754002898 -27274.3775402898 -27274.377540865 -27274.37754101662 -27274.37754101662 -27274.37754004213 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.3775410865 -27274.3775410875 -27274.3775410875 -27274.3775410875 -27274.3775410875 -27274.3775410875 -27274.3775410875 -27274.37754138718 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754246895 -27274.37748754261 -27274.37748754261 -27274.37748754261 -27274.37748754261
	SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF SCF	<pre>converged c</pre>	atth 4 a thus a a thus a a a a a a a a a a a a a a a a a a a	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 41\\ 41\\ 0.02\\ 20\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41\\ 41$	Final Final	energy energy 200 8 1.0.0 energy		-27274.37752144962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.377538437 -27274.37753839733 -27274.37753808531 -27274.37753908531 -27274.37753966563 -27274.37754022898 -27274.3775402898 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.3775401865 -27274.3775401865 -27274.3775401865 -27274.3775401865 -27274.37754084213 -27274.37754108751 -27274.37754108751 -27274.37754108751 -27274.37754138718 -27274.37754335791 -27274.37754335791 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.377543978102 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.377543754395899 -27274.377543754357125 -27274.377543754395899 -27274.377543754357125 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754395899 -27274.377543754357125 -27274.377543754357125 -27274.377543754357125 -27274.377543754357125 -27274.377543754357125 -27274.377543754357125 -27274.377543754325
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 616\\ 617\\ 618\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 629\\ 633\\ 634\\ 635\\ 636\\ 637\\ 638\\ 639\\ 639\\ 640\\ \end{array}$	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a a thuit a a a a a a a a a a a a a a a a a a a	iteration iteration on f F del 5 1.(iteration	411 411	Final Final	energy energy		-27274.37752144962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.377538437 -27274.37753839733 -27274.37753908531 -27274.37753908531 -27274.37753906563 -27274.37754022898 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754084213 -27274.37754084213 -27274.37754108751 -27274.37754138718 -27274.37754138718 -27274.37754042695 -27274.37754042695 -27274.37754335791 -27274.377543754367125 -27274.37754375454261 -27274.377543754367125 -27274.377543754367125 -27274.37754375486
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a a the feature of the second se	iteration iteration of f f del f 1.(iteration	411 (0) 411	Final Final	energy energy 1.00 8 1.00 energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.37753839733 -27274.37753839733 -27274.37753908531 -27274.37753908531 -27274.37754040643 -27274.37754040643 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.3775401692 -27274.37754108962 -27274.37754116962 -27274.3775418718 -27274.37754246896 -27274.3775402695 -27274.3775402695 -27274.3775402695 -27274.3775402695 -27274.37749776102 -27274.37749776102 -27274.37754367125 -27274.37754367125 -27274.37754367125 -27274.37754307486 -27274.3775428152
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	converged conve	a a the feature of the second se	iteration iteration on f F del 5 1.(iteration	411 (0) 411	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.37753749272 -27274.3775384357 -27274.37753839733 -27274.37753908531 -27274.37753908531 -27274.3775400643 -27274.3775400643 -27274.3775400643 -27274.3775406585 -27274.37754101662 -27274.37754101662 -27274.377541046213 -27274.37754104751 -27274.37754104751 -27274.37754106751 -27274.37754138718 -27274.37754138718 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754335791 -27274.37754395899 -27274.37748754261 -27274.37754395899 -27274.377543957125 -27274.377543077486 -27274.377543077486 -27274.377543077486 -27274.377543267125 -27274.377543267125 -27274.377543428152 -27274.37754428152 -272
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 620\\ 622\\ 623\\ 622\\ 623\\ 624\\ 625\\ 626\\ 626\\ 627\\ 638\\ 639\\ 630\\ 631\\ 632\\ 638\\ 639\\ 639\\ 639\\ 639\\ 640\\ 641\\ 643\\ \end{array}$	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	converged interm > 1.6627 converged	a a the result of the second s	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 0 \\ 2 \\ 1 \\ 4 \\ 4 \\ 1 \\ 1 \\ 4 \\ 4 \\ 4 \\ 1 \\ 1$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.3775384377 1.0623435 -27274.37753839733 -27274.37753839733 -27274.37753908531 -27274.37753906563 -27274.37753966563 -27274.37754022898 -27274.37754022898 -27274.3775402898 -27274.3775402898 -27274.37754016865 -27274.37754101662 -27274.37754084213 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.3775410865 -27274.3775410875 -27274.37754138718 -27274.37754338791 -27274.3775420896 -27274.37754428192 -27274.37754428192 -27274.37754418491 -27274.37754418491
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a a the function of the second s	iteration iteration of f f del of f f del of f del	$\begin{array}{c} 411\\ 441\\ 0\\ 0\\ 2\\ 1\\ 411\\ 411\\ 411\\ 411\\ 411\\ 411\\ 41$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.3775389437 -27274.3775389733 -27274.3775389733 -27274.37753908531 -27274.37754040643 -27274.37754040643 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.3775401662 -27274.3775401662 -27274.377541046213 -27274.37754104613 -27274.37754104751 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.3775410965 -27274.37754246896 -27274.3775402695 -27274.377540276 -27274.377540786 -27274.377540786 -27274.377540786 -27274.
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a a a r 4 a a a a a a a a a a a a a a a	iteration iteration of f f del 5 1.(iteration	$\begin{array}{c} 41\\ 41\\ 0\\ 0\\ 2\\ 1\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\ 4\\$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.37753839733 -27274.37753839733 -27274.37753906531 -27274.37753966563 -27274.37754040643 -27274.37754040643 -27274.37754015865 -27274.37754015865 -27274.3775401662 -27274.3775401662 -27274.37754104751 -27274.3775410662 -27274.37754106751 -27274.37754116865 -27274.37754108751 -27274.37754108751 -27274.37754108751 -27274.37754108751 -27274.37754108751 -27274.37754108751 -27274.37754108751 -27274.37754335791 -27274.37754335791 -27274.37754395899 -27274.37754395899 -27274.377543077486 -27274.377543077486 -27274.37754109361 -27274.37754461948
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 616\\ 617\\ 618\\ 620\\ 621\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 630\\ 631\\ 632\\ 633\\ 634\\ 635\\ 636\\ 637\\ 638\\ 639\\ 640\\ 641\\ 642\\ 643\\ 644\\ 645\\ 646\\ 646\\ 646\\ 646\\ 646\\ 646$	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	converged interm 1.6627 converged c	a a a r 4 a a a a a a a a a a a a a a a	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 0 \\ 2 \\ 1 \\ 4 \\ 4 \\ 1 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.37753749272 -27274.3775384357 -27274.37753839733 -27274.37753808531 -27274.37753906553 -27274.37753966563 -27274.3775400643 -27274.37754002898 -27274.377540643 -27274.3775406865 -27274.37754101662 -27274.37754101662 -27274.377541046213 -27274.37754104751 -27274.37754104751 -27274.37754104751 -27274.3775410695 -27274.37754138718 -27274.377542896 -27274.377542896 -27274.377542895 -27274.377542895 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.377543957486 -27274.3775440265 -27274.3775440265 -27274.3775440276 -27274.37754409361 -27274.3775440948 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -27274.3775440044 -2727
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a a a r 4 a a a a a a a a a a a a a a a	iteration iteration of f del 5 1.0 iteration	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 0 \\ 2 \\ 1 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4$	Final Final	energy energy		-27274.3775314962 -27274.3775314962 -27274.37753749272 -27274.3775384377 1.0623435 -27274.37753839733 -27274.37753808531 -27274.37753908531 -27274.37753966563 -27274.37754022898 -27274.37754022898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.37754016662 -27274.3775401662 -27274.3775401662 -27274.3775401662 -27274.37754016751 -27274.37754104751 -27274.37754104751 -27274.3775410865 -27274.3775410875 -27274.3775410875 -27274.37754318718 -27274.37754335791 -27274.37754335791 -27274.37754335791 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.37754395899 -27274.3775440265 -27274.3775440265 -27274.3775440845 -27274.3775440845 -27274.3775440845 -27274.377544084 -27274.377544084 -27274.3775440946 -27274.377544084 -27274.3775440946
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	converged interm 1.662; converged co	a a a r 4 a a a a a a a a a a a a a a a	iteration iteration of f f del f 1.(iteration	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 0 \\ 2 \\ 1 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4$	Final Final	energy energy		27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.37753839733 -27274.37753808531 -27274.37753908531 -27274.37754040643 -27274.37754040643 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.3775401662 -27274.3775401662 -27274.37754104751 -27274.37754104751 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.37754116962 -27274.37754246896 -27274.37754246896 -27274.3775404213 -27274.3775402895 -27274.3775402895 -27274.3775402895 -27274.3775407485 -27274.3775407486 -27274.3775409312 -27274.37754109361 -27274.3775400144 -27274.3775400123 -27274.3775400144 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.3775400123 -27274.37754003123
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	converged conven	a a a r 4 a a a a a a a a a a a a a a a	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 0 \\ 2 \\ 1 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.37753749272 -27274.3775384357 -27274.37753839733 -27274.37753908531 -27274.37753908531 -27274.3775400643 -27274.3775400643 -27274.37754022898 -27274.3775401653413 -27274.37754018685 -27274.3775401662 -27274.3775401662 -27274.37754104751 -27274.37754104751 -27274.37754116962 -27274.377541697 -27274.377541697 -27274.377541287 -27274.377541287 -27274.377541287 -27274.377541287 -27274.377541287 -27274.377541287 -27274.377541287 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754261 -27274.37754261 -27274.37754261 -27274.37754268 -27274.3775440295 -27274.37754408152 -27274.3775440941 -27274.37754609415 -27274.377546075
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	converged interm > 1.6627 converged	a a a r 4 a a a a a a a a a a a a a a a	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 411 \\ 0 \\ 0 \\ 2 \\ 1 \\ 1 \\ 41 \\ 41 \\ 41 \\ 41 \\ 41 \\ $	Final Final	energy energy		-27274.37753144962 -27274.37753749272 -27274.37753749272 -27274.37753749272 -27274.3775384357 -27274.37753839733 -27274.37753808531 -27274.37753908531 -27274.37753906563 -27274.37754022898 -27274.37754022898 -27274.37754022898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775402898 -27274.3775401662 -27274.3775401662 -27274.37754104751 -27274.37754104751 -27274.3775410875 -27274.3775418718 -27274.3775418718 -27274.377542898 -27274.377542898 -27274.377542898 -27274.377542898 -27274.3775428152 -27274.3775402695 -27274.3775400315 -27274.3775460341
	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a aa r 14 a aa a aa a	iteration iteration of f f del of f del de f del del de f del del de f del del de f del del del de f del del del del del del del del del del	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 0 \\ 2 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4$	Final Final	energy en		27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.3775389437 -27274.3775389733 -27274.3775389733 -27274.37753908531 -27274.37754040643 -27274.37754040643 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.37754015865 -27274.3775401662 -27274.3775401662 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754084213 -27274.37754042695 -27274.37754042695 -27274.37754042695 -27274.37754042695 -27274.37754042695 -27274.37754042695 -27274.37754402695 -27274.37754609415 -27274.37754609
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 620\\ 622\\ 623\\ 622\\ 623\\ 622\\ 622\\ 623\\ 622\\ 625\\ 626\\ 627\\ 638\\ 639\\ 630\\ 633\\ 634\\ 638\\ 639\\ 640\\ 641\\ 642\\ 643\\ 644\\ 645\\ 646\\ 647\\ 648\\ 649\\ 650\\ 651\\ 651\\ 652\\ 652\\ 653\\ 852\\ 653\\ 655\\ 653\\ 655\\ 655\\ 655\\ 655\\ 655$	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a a a r 4 a a a a a a a a a a a a a a a	iteration iteration of nf F del 5 1.(iteration	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 2 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.37753749272 -27274.377538435 -27274.37753839733 -27274.3775383174 -27274.37753906531 -27274.3775400643 -27274.3775400643 -27274.37754016865 -27274.37754016865 -27274.37754016865 -27274.3775401662 -27274.3775401662 -27274.3775401662 -27274.37754104751 -27274.37754104751 -27274.3775416962 -27274.3775416962 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754335791 -27274.37754335791 -27274.37754367125 -27274.3775402895 -27274.37754367125 -27274.3775406945 -27274.3775400140 -27274.3775400140 -27274.3775400140 -27274.37754603123 -27274.37754254067 -27274.37754254067 -27274.37754260915 -27274.37754254067 -27274.37754254067 -27274.37754254067 -27274.37754254067 -27274.37754254067 -27274.37754254067 -27274.37754254067 -27274.37754560194 -27274.37754560194 -27274.37754560194 -27274.377545601932
$\begin{array}{c} 611\\ 612\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 620\\ 622\\ 623\\ 624\\ 625\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 637\\ 638\\ 639\\ 630\\ 631\\ 635\\ 636\\ 637\\ 638\\ 639\\ 640\\ 641\\ 642\\ 643\\ 644\\ 648\\ 649\\ 650\\ 651\\ 652\\ 653\\ 654\\ \end{array}$	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a aa r 4 a a a a a a a a a a a a a a a a	iteration iteration on f F del 5 1.(iteration	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 0 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.37753749272 -27274.3775384357 -27274.37753839733 -27274.37753906531 -27274.37753906531 -27274.3775400643 -27274.3775400643 -27274.3775406543 -27274.3775406543 -27274.37754101662 -27274.37754101662 -27274.37754104751 -27274.37754104751 -27274.377541662 -27274.377541662 -27274.377541662 -27274.377541662 -27274.3775416751 -27274.3775416751 -27274.3775416751 -27274.3775416751 -27274.3775416751 -27274.37754246896 -27274.37754246896 -27274.37754246896 -27274.37754395899 -27274.37754395899 -27274.377543071486 -27274.37754109312 -27274.37754109361 -27274.3775440276 -27274.3775440945 -27274.3775440945 -27274.37754500144 -27274.37754610945 -27274.37754610945 -27274.37754609415 -27274.37754609415 -27274.37754609415 -27274.37754609415 -27274.37754609415 -27274.37754609415 -27274.37754609415 -27274.37754609322 -27274.3775460932
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	SCFF SCFF SCFF SCFF SCFF SCFF SCFF SCFF	<pre>converged c</pre>	a aa r 4 a a a a a a a a a a a a a a a a	iteration iteration of f f del of f del del del f del	$\begin{array}{c} 4 \\ 4 \\ 4 \\ 0 \\ 2 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4$	Final Final	energy energy		-27274.3775314962 -27274.37753749272 -27274.37753749272 -27274.377538437 -27274.3775389733 -27274.3775389733 -27274.37753908531 -27274.37753908531 -27274.3775400643 -27274.37754002898 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.37754018665 -27274.3775401867 -27274.3775401867 -27274.3775401867 -27274.3775401867 -27274.3775401875 -27274.3775401875 -27274.3775401875 -27274.3775401875 -27274.3775402895 -27274.377540895 -27274.37754087125 -27274.3775408125 -27274.3775408125 -27274.3775408125 -27274.3775408123 -27274.3775408123 -27274.37754609415 -27274.3

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658		
	658 SCF converged at iteration 41 Final energy = -27274.37754439248	
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661	661 SCF converged at iteration 41 Final energy = -27274.37754610373	
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004	oof sor converged at the attent of Final energy2/2/4.3/75401036/	
665	505 SCF converged at iteration 41 Final energy = -2/2/4.3/15461026/	
666	666 interm rho nf F del 0.000100000 137 -27274.377 546 108 1 -0.	000 007 670 4
667	667 :::> 1.6853380 1.0025643 1.0865944 1.1572454	
668	668 SCF converged at iteration 41 Final energy = -27274.37754610732	
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087	unterm rno ni r del 0.000010000 156 -27274.377 546 109 4 -0.	000 000 001 3
688	b88 :::> 1.6849066 1.0025845 1.0874081 1.1585546	
689	689 SCF converged at iteration 41 Final energy = -27274.37754610938	
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692	692 SCF converged at iteration 41 Final energy = -27274.37754610938	
693	693 SCF converged at iteration 41 Final energy = -27274 37754610911	
694	694 SCF converged at iteration 41 Final energy = -27274 37754610940	
605	605 SCF converged at iteration (1 Final energy = -27274 37754610917	
606	606 SOF converged at iteration 41 Final anergy =	
607	307 soft converged at iteration 41 Final energy - -27274.37754010942	
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699	SCF converged at iteration 41 Final energy = -2/2/4.3//54610939	
700	SCF converged at iteration 41 Final energy = -27274.37754610930	
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703	703 SCF converged at iteration 41 Final energy = -27274.37754610940	
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707	707 At the return from NEWUOA number of function values = 173	
707 708	707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942	
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707 708 709 710	707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 709 1.0025849 709 1.1585570	
707 708 709 710 711	707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 1.0874118 710 New parameters are 711 3.2777475F-00 3.2777475F-00 1.6626263F+00 5.3795715F+00 1.6670872F+00	
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707 708 709 710 711 712 712	707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 710 New parameters are 711 3.2777475E-02 1.8626263E+00 712 SCF converged at iteration 41 Final energy = -27274.37754610942	
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$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ \end{array}$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	55+ 65+ 75+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.04529E-03 1.9084131E-01 .5938581E-04 -1.042761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ \end{array}$	1000 7077 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 1.0874118 1.1585570 710 New parameters are 1.0874118 1.1585570 711 S.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 712 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 713 15 15+ 25+ 38+ 48+ 715 15+ 25+ 38+ 48+ 716 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 718 .2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 720 6.1052208E-02 -2.7212503E-06 -2.4451140E-05 2.5997072E-04 -5.7257873E-04 3 721 1.1317780E-01 6.4661788E-06 5.8087512E-05 -6.1594002E-004 1.3479664E-03 7 722 2.1181678E-01 -1.17768698E-05 1.0570257E-04<	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 8.9549947E-05 2.0217706E-04 7.7763953E-01 8.6084676E-04 -1.8505829E-03 1.9084131E-01 8.95851E-04 -1.0442761E-02 4.35094499E-01 2.148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.5322441E-01
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724 \end{array}$	1007 707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 700 New parameters are 711 3.2777475E-02 712 3.2777475E-02 714 -27274.37754610942 715 1.6670872E+00 716 -27274.37754610942 717 5 714 15+ 715 15+ 716 -4.1678552E+03 717 717 718 3.2777475E-02 719 3.2777475E-02 719 3.2777475E-02 717 717 718 5 719 3.2777475E-02 719 3.2777475E-02 717 718 3.2777475E-02 719 3.2777475E-02 710 1.57309076E-06 711 1.371780E-01 712 1.1371780E-01 713 1.1371780E-01 714 1.185370E-03<	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 8.9549947E-05 2.0217706E-04 7.7763953E-01 8.094676E-04 -1.8505829E-03 1.9084131E-01 5.938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718644E-01 -3.322441E-01 .1094051E-02 -6.2243418E-01 -3.3766148E-01
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ \end{array}$	1007 707 708 709 709 709 709 709 709 709 709 709 709	55+ 65+ 75+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1094051E-02 -6.2243418E-01 -3.3766148E-01 .6524111E-01 4.7977497E-01 2.0741439E-01
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ \end{array}$	1007 707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 1.0874118 1.1585570 710 New parameters are 1.0874118 1.1585570 711 S.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 712 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 713 15+ 25+ 35+ 45+ 716 15+ 25+ 35+ 45+ 717 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 1 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 1 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 718 -4.1678552E+03 -7.3099076E-06 -6.1014939E-05 1.3503449E-04 -8 720 6.1052208E-02 -2.7212503E-06 -2.4451140E-05 2.5997072E-04 -5.757873E-03 -7	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 8.9549947E-05 2.0217706E-04 7.7763953E-01 8.084676E-04 -1.850529E-03 1.9084131E-01 8.95851E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1094051E-02 -6.2243418E-01 -3.3766148E-01 .6524111E-01 4.7977497E-01 2.0741439E-01 .052865E-00 1.0136423E+00 3.4555769E-01
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ 725\\ 726\\ 727\\ \end{array}$	1007 707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 1.0874118 1.1585570 709 1.6848935 1.0025849 1.0874118 1.1585570 700 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 711 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 714 15+ 25+ 35+ 45+ 714 15+ 25+ 35+ 45+ 716 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 7 6.1052208E-02 -2.7212503E-06 -2.4451140E-05 2.5997072E-04 -5.7257873E-04 3 721 1.1371780E-01 6.4661788E-06 5.8087512E-05 -6.1594002E-04 1.3479564E-03 -7 723 3.945421E-01 1.376668E-05 1.0570257E-04 1.1185370E-03 3.9079496E-03 -1 724 7.3499994E-01 -2.7775219E	55+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 2.9549947E-05 2.0217706E-04 7.7763953E-01 3.0684676E-04 -1.8505829E-03 1.9084131E-01 3.9538581E-04 -1.0442761E-02 4.3509449E-01 .2618495E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1094051E-02 -6.2243418E-01 -3.3766148E-01 .052865E+00 1.0136423E+00 3.455769E-01 .02336517E-01 1.2190063E-01 4.7160748E-02
$\begin{array}{c} 707\\ 708\\ 709\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ 727\\ 728 \end{array}$	1007 707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 1.0874118 1.1585570 700 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 712 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 713 15+ 25+ 35+ 45+ 716 15+ 25+ 35+ 45+ 717 15+ 15+ 25+ 35+ 45+ 718 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 719 3.2777475E-02 6.3766410E-07 5.7309076E-04 1.1185370E-03 3.7907496E-03 -1 721 1.1181678E-01 -1.1776869E-05 -1.0570	55+ 65+ 75+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1094051E-02 -6.223418E-01 -3.3766148E-01 .0628665E+00 1.0136423E+00 3.4555769E-01 .2336517E-01 1.2190063E-01 -2.333230E-01 .2574109E+00 -7.1892239E-01 -2.333230E-01
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ 727\\ 728\\ 728\\ 729\\ 728\\ 729\\ \end{array}$	1007 707 At the return from NEWUOA number of function values = 173 708 F= -27274.37754610942 709 1.6848935 1.0025849 1.0874118 1.1585570 700 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 712 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 713 15+ 25+ 35+ 45+ 714 15+ 25+ 35+ 45+ 714 -4.1678552E+03-7.8202739E+02-1.9970482E+02 -5.2155429E+01-1 1 717 8 -4.1678552E+03-7.8202739E+02-1.9970482E+02 -5.2155429E+01-1 717 18 -4.1678552E+03-7.8202739E+02-1.9970482E+02 -5.2155429E+01-1 717 11 -4.1678552E+03-7.8202739E+02-1.9970482E+02 -5.2155429E+01-1 -7.22 720 6.1052208E-02-2.7212503E-06 -2.4451140E-05 2.5997072E-04 -5.3757873E-04 -7.22 721 1.1371780E-01 -6.4661788E-06 1.6806127E-04 -1.18570E-03 -7.22 722 2.1181678E-01	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 3.9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505822E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2018495E-04 -7.3718664E-01 -3.3766148E-01 .602865E-00 1.0136423E+00 3.4555769E-01 .062865E5E-00 1.2190063E-01 4.7160748E-02 .25674109E+00 -7.1892239E-01 -2.333230E-01 .1418558E-01 -2.6643338E-01 -8.270513E-02
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 715\\ 716\\ 717\\ 718\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ 727\\ 728\\ 729\\ 730\\ \end{array}$	At the return from NEWUQA number of function values = 173 F= -27274.37754610942 1.6848935 1.0025849 1.0874118 1.1585570 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 13 714 715 15+ 25+ 35+ 45+ 716 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 718 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 720 6.1052208E-02 -2.7212503E-06 -2.4451140E-05 2.5997072E-04 -5.7257873E-04 3 721 1.1371780E-01 6.4661788E-06 5.8087512E-05 -6.1594002E-04 1.3479564E-03 -7 722 2.1181678E-01 -1.1776869E-05 -1.0570257E-04 1.763196E-03 -2.4045368E-03 1 723 3.9455421E-01 1.8779658E-05 -1.058612F-04 -1.763196E-03 -5.2448412E-03 2 725 1.3694267E+00 3.9581146E-05 3.5469575E-04 -3.6690519E-03 6.526712E-03 1 726 2.5522453E+00 -5.5531012E-05 -5.0644472E-04 4.8195743E-03 -1.3768212E-02 1 727 4.7592004E+00 7.5042533E-05 6.7454424E-04 -6.6652007E-03 -1.3640398E-01 1 728 8.8821010E+00 -9.9650704E-05 -8.8184744E-04 1.1265810E-02 -9.1814825E-01 -1 729 1.659858E+01 1.377180E-04 1.4607049E-03 7.8986582E-05 1.5840398E-01 1 729 1.659828E+01 1.3791887-04 1.4607049E-03 7.8898658E-05 1.5840398E-01 1 729 1.659828E+01 1.3791887-04 1.4607049E-03 7.8898658E-05 1.5840398E-01 1 729 1.659828E+01 1.3791887-04 1.4607049E-03 6.1058012E-02 -5.7101352E-01 -5 730	55+ 65+ 75+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 2.9549947E-05 2.0217706E-04 7.7763953E-01 3.0684676E-04 -1.8505829E-03 1.9084131E-01 5.938581E-04 -1.0442761E-02 4.3509449E-01 .2618495E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1094051E-02 -6.2243418E-01 -3.3766148E-01 .052865E+00 1.0136423E+00 3.455769E-01 .2336517E-01 1.2190063E-01 4.7160748E-02 .2574109E+00 -7.189239E-01 -2.33330E-01 .1418558E-01 2.26643838E-01 8.2270513E-02 .6179744E-01 2.666414E-01 8.2644473R-02
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 715\\ 716\\ 717\\ 718\\ 720\\ 721\\ 722\\ 723\\ 724\\ 722\\ 723\\ 724\\ 726\\ 727\\ 728\\ 729\\ 730\\ 731\\ \end{array}$	1007 707 At the return from NEWUOA number of function values = 173 708 F = -27274.37754610942 709 1.6848935 1.0025849 1.0874118 1.1585570 700 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 712 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 713 15+ 25+ 35+ 45+ 716 15+ 25+ 35+ 45+ 717 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 717 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 718 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 717 -1.1371780E-01 6.4661788E-06 5.8087512E-05 -6.1594002E-04 -1.879542E+03 -1.37949564E-03 -1.73499994E+01 -1.77519E-05 -2.4890013E-04 -6.652007E-03 -5.248412E-03 -2.2652453E+00 -5.5531012E-05 -5.0644472E-04 -6.6562007E-03 -5.265412E-03 -1.769204E+00 -5.55310	55+ 65+ 75+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1094051E-02 -6.224318E-01 -3.3766148E-01 .062665E+00 1.0136423E+00 3.4555769E-01 .2336517E-01 1.2190063E-01 -2.333230E-01 .2574109E+00 -7.1892239E-01 -2.333230E-01 .1418558E-01 -2.66643838E-01 -8.2270513E-02 .6179744E-01 2.666146E-01 8.264473E-02 .733316E-01 -1.844320E-01 6.7834903R-02
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$\begin{array}{c} 707\\ 708\\ 709\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 726\\ 727\\ 728\\ 726\\ 727\\ 728\\ 730\\ 731\\ 732\\ 732 \end{array}$	1007 707 708 709 709 709 709 709 709 709 709 709 709	55+ 65+ 75+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1094051E-02 -6.2243418E-01 -3.3766148E-01 .6524111E-01 4.7977497E-01 2.0741439E-01 .062865E+00 1.0136423E+00 3.455769E-01 .2336517E-01 1.2190063E-01 4.7160748E-02 .2574109E+00 -7.1892239E-01 2.3332330E-01 .418558E-01 -2.6643838E-01 8.264473E-02 .6179744E-01 2.666446E-01 8.264473E-02 .6138740E-01 2.1834120E-01 6.7834903E-02 .7333116E-01 2.1834120E-01 6.7834903E-02 .6052348E-02 -3.3602641E-02 1.049887E-02
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$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 715\\ 716\\ 717\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ 728\\ 729\\ 730\\ 731\\ 732\\ 733\\ 734\\ 735\\ 736\\ 737\\ 738\\ 737\\ 738\\ \end{array}$	At the return from NEWUOA number of function values = 173 707 At the return from NEWUOA number of function values = 173 708 F = -27274.37754610942 709 1.6848935 1.0025849 1.0874118 1.1585570 710 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 712 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 713 15+ 25+ 35+ 45+ 716 15+ 25+ 35+ 45+ 717 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 718 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+03 -3 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.194002E-04 -1.87378E-04 3 721 1.181678E-02 -2.7212503E-06 -2.445140E-05 2.5997072E-04 1.34799564E-03 -1	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2148510E-03 -2.1151300E-01 -3.3766148E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .652411E-01 4.7977497E-01 2.33230E-01 .652411E-01 4.7977497E-01 -2.33230E-01 .2574109E-00 -7.189239E-01 -2.33230E-01 .2574109E-00 -7.89239E-01 -2.33230E-01 .1418558E-01 -2.6643838E-01 8.264473E-02 .6179744E-01 2.8866146E-02 -1.049987E-02 .6052348E-02 -3.3602641E-02 -1.049887E-02 .7912344E-01 -8.359590E-02 -2.4663349E-02 .2191235E-02 -3.644666E-02 -1.31440E-02 .2962445E-03 -1.5389625E-03 -4.5630116E-04 .90667614E-02 8.7101348E-03
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ 727\\ 725\\ 726\\ 727\\ 735\\ 736\\ 737\\ 735\\ 736\\ 737\\ 738\\ 738\\ 739\\ \end{array}$	At the return from NEWUQA number of function values = 173 F = -27274.37754610942 709 1.6848935 1.6848935 1.6848935 1.6848935 3.2777475E-02 3.2777475E-02 3.2777475E-02 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 713 714 715 1.5+ 2.5+ 3.2777475E-02 6.105208E-02 2.27212503E-06 722 1.1371780E-01 6.4661788E-06 1.6870512E-05 1.1371780E-01 6.4661788E-06 1.188678E-03 1.3875421E-01 1.3879548E-03 1.387562E+01 1.387562E+01 1.38769658E-05 1.6806127E-04 7.349994E-01 2.7775218E-05 3.0455421E-01 1.38797849E-03 1.3971	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505828E-03 1.9084131E-01 .538581E-04 -1.0442761E-02 4.3509449E-01 .2184501E-03 2.1151300E-01 -4.1956006E-01 .208495E-04 -7.3718664E-01 -3.3766148E-01 .6028665E-00 1.0136423E+00 3.4555769E-01 .02386517E-01 1.2190063E-01 4.7160748E-02 .236517E-01 1.2190063E-01 4.7160748E-02 .236517E-01 1.2190063E-01 8.2270513E-02 .6179744E-01 2.6866146E-01 8.2644473E-02 .615234E0-01 2.1834120E-01 6.7834903E-02 .615234E0-01 2.834595950E-02 -2.4606349E-02 .7912344E-01 8.0359590E-02 -2.4606349E-02 .2962445E-02 3.6463965EE-03 -1.133140E-03 .2962445E-03 3.56332E-03 2.5765332E-03 .9030766E-02 8.7101348E-03 2.6628490E-03 .9030766E-02 5.6108718E-03
$\begin{array}{c} 707\\ 708\\ 709\\ 710\\ 711\\ 712\\ 713\\ 714\\ 715\\ 716\\ 717\\ 718\\ 719\\ 720\\ 721\\ 722\\ 723\\ 724\\ 725\\ 726\\ 727\\ 728\\ 729\\ 731\\ 732\\ 731\\ 732\\ 733\\ 734\\ 735\\ 736\\ 737\\ 738\\ 739\\ 740\\ 740\\ 740\\ 740\\ 740\\ 740\\ 740\\ 740$	At the return from NEWUOA number of function values = 173 F= -27274.37754610942 Top 1.6848935 1.0025849 1.0874118 1.1585570 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 S2 S2 S2 S2 S2	55+ 6S+ 75+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 2.9549947E-05 2.0217706E-04 7.7763953E-01 3.0684676E-04 -1.8505829E-03 1.9084131E-01 5.938581E-04 -1.0442761E-02 4.3509449E-01 .2618495E-04 -7.3718664E-01 -3.5322441E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .094051E-02 -6.2243418E-01 -3.3766148E-01 .052865E+00 1.0136423E+00 3.455769E-01 .052865E+00 1.01369239E-01 -2.333230E-01 .274149E+00 -7.189239E-01 -2.333230E-01 .21834120E-01 6.7834903E-02 .37033116E-01 .6179744E-01 2.8665146E-01 8.264473E-02 .6179744E-01 2.86590E-02 -2.466349E-02 .7333116E-01 2.1834120E-01 6.7834903E-02 .7333116E-01 2.1834120E-01 6.7834903E-02 .2191235E-02 -3.6464966E-02 -1.1231440E-02 .2191235E-02 -3.6464966E-02 -1.231440E-02 .2191235E-02 -5.6108718E-03<
707 708 709 710 712 713 714 715 716 717 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 737 738 739 730 738 739 730	At the return from NEWUQA number of function values = 173 F = -27274.37754610942 709 1.6848935 1.08284935 1.08284935 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 713 714 715 716 717 718 719 3.2777475E-02 6.1052208E-02 7.2122503E-06 7.1181678E-01 7.1181678E-01 7.22 7.1181678E-01 7.339934E-01 7.77722 7.1181678E-01 7.349994E-01 7.77519E-05 7.3690174E-04 7.36994267E+00 7.36994267E+00 7.36994267E+00 7.349994E-01 7.777519E-05 7.3660519E-03 7.55204512E-04 7.55204512E-04 7.55204512E-04 7.5622453E+00 </th <th>5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .6944947E-05 2.0217706E-04 7.7763953E-01 .6094676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .652411E-01 4.7977497E-01 2.0741439E-01 .65265E+00 1.0136423E+00 3.4555769E-01 .2336517E-01 1.2190063E-01 4.7160748E-02 .2574109E+00 -7.819239E-01 -2.332330E-01 .4148558E-01 -2.6664383E-01 -8.2470513E-02 .6179744E-01 2.6666146E-01 8.2644473E-02 .6052348E-02 -3.3002641E-02 -1.049987E-02 .733116E-01 2.3389590E-02 -2.466349E-02 .2962445E-03 -1.5389625E-03 -4.5630116E-04 .2962645E-03 -1.5389625E-03 -2.65324E-03 .9030766E-02 8.39402922E-03 2.5765332E-03 .9030766E-02 8.3103362E-03<</th>	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .6944947E-05 2.0217706E-04 7.7763953E-01 .6094676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .652411E-01 4.7977497E-01 2.0741439E-01 .65265E+00 1.0136423E+00 3.4555769E-01 .2336517E-01 1.2190063E-01 4.7160748E-02 .2574109E+00 -7.819239E-01 -2.332330E-01 .4148558E-01 -2.6664383E-01 -8.2470513E-02 .6179744E-01 2.6666146E-01 8.2644473E-02 .6052348E-02 -3.3002641E-02 -1.049987E-02 .733116E-01 2.3389590E-02 -2.466349E-02 .2962445E-03 -1.5389625E-03 -4.5630116E-04 .2962645E-03 -1.5389625E-03 -2.65324E-03 .9030766E-02 8.39402922E-03 2.5765332E-03 .9030766E-02 8.3103362E-03<
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707 708 709 710 712 713 714 715 716 717 719 720 721 722 723 724 725 726 727 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 730 738 739 730 738 734 737 741	At the return from NEWUQA number of function values = 173 F = -27274.37754610942 709 1.6848935 1.6848935 3.2777475E-02 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 713 714 715 15+ 25+ 716 717 718 719 3.2777475E-02 6.1052208E-02 7.2121503E-06 7.309076E-06 6.1052208E-02 7.21181678E-01 1.1371780E-01 6.4661788E-06 722 1.181678E-01 7.3499994E-01 7.777519E-05 7.3660519E-03 7.369070F2E-04 7.389994E-01 7.3777518E-04 7.389994E-01 7.777519E-05 7.389949704 7.5520453E+00 7.5520453E+01 7.59204E+00 </th <th>5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505825E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2018495E-04 -7.3718664E-01 -3.3766148E-01 .6524111E-01 4.7977497E-01 2.0741439E-01 .65265E+00 1.0136423E+00 3.4555769E-01 .2336517E-01 1.2190063E-01 -4.760748E-02 .6526411E-01 -2.664338E-01 -8.2270513E-02 .6179744E-01 2.6666146E-01 8.264473E-02 .6152348E-02 -3.3302641E-02 -1.049987E-02 .7912344E-01 -8.0359500E-02 -2.4666349E-02 .2962445E-03 -1.5339625E-03 -4.5633116E-04 .99630766E-02 8.7101348E-03 2.628490E-03 .9030766E-02 8.7103426E-03 1.718714E-03 .5038816E-03 3.3103362E-03 1.718714E-03 .5038816E-03 3.3103362E-03<!--</th--></th>	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505825E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2018495E-04 -7.3718664E-01 -3.3766148E-01 .6524111E-01 4.7977497E-01 2.0741439E-01 .65265E+00 1.0136423E+00 3.4555769E-01 .2336517E-01 1.2190063E-01 -4.760748E-02 .6526411E-01 -2.664338E-01 -8.2270513E-02 .6179744E-01 2.6666146E-01 8.264473E-02 .6152348E-02 -3.3302641E-02 -1.049987E-02 .7912344E-01 -8.0359500E-02 -2.4666349E-02 .2962445E-03 -1.5339625E-03 -4.5633116E-04 .99630766E-02 8.7101348E-03 2.628490E-03 .9030766E-02 8.7103426E-03 1.718714E-03 .5038816E-03 3.3103362E-03 1.718714E-03 .5038816E-03 3.3103362E-03 </th
707 708 709 710 712 713 714 715 716 717 715 716 717 721 722 723 724 725 726 727 728 729 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 730 731 732 733 734 735 736 736 737 738 739 730 731 732 733 734 735 736 736 737 738 739 730 731 732 733 734 735 736 737 736 737 736 737 737 738 739 730 731 732 733 734 735 736 737 734 735 736 737 737 737 738 739 730 731 732 733 734 735 736 737 737 734 735 736 737 737 737 737 737 737 737 737 737	At the return from NEWUQA number of function values = 173 F = -27274.37754610942 1.6848935 1.0025849 1.0874118 1.1585570 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 714 15+ 25+ 35+ 45+ 716 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 1 15+ 25+ 35+ 45+ 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 8 720 2.1181678E-01 -1.177689E-05 -1.0570257E-04 -1.3479564E-03 -7 721 1.3317380E-01 -2.4059013E-04 -2.6020802E-03 -5.2448412E-03 2 723 1.3694267E+00 3.9681146E-05 3.669512E-04 -3.6690512E-03 -1.3768212E-02 1 724 4.592004E+00 7.5042533E	55+ 65+ 78+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 2.9549947E-05 2.0217706E-04 7.7763953E-01 2.094676E-04 -1.8505829E-03 1.9084131E-01 5.938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.371664E-01 -3.3766148E-01 .6524111E-01 4.7977497E-01 2.0741439E-01 .052865E-00 1.013664221-00 3.4555769E-01 .2336517E-01 1.2190063E-01 4.7160748E-02 .65294111E-01 2.1834120E-01 6.7834903E-02 .6179744E-01 2.6643388E-01 8.2270513E-02 .6179744E-01 2.664348502 -1.134407E-02 .6052348E-02 -3.3602641E-02 -1.1049887E-02 .7912344E-01 -8.0359590E-02 -2.4606349E-02 .21962445E-03 -1.5389625E-03 -4.5630116E-04 .2962445E-03 -3.10348E-03 2.676332E-03 .9030766E-02 8.3103362E-03 1.0152861E-03 .903816E-03 3.3103362E-03
707 708 709 710 712 713 714 715 716 715 716 717 722 723 724 722 723 724 725 726 727 728 729 724 725 726 727 728 729 731 731 732 733 734 735 736 737 733 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 737 737 734 735 736 737 734 735 736 737 737 734 737 734 737 734 737 737 737	At the return from NEWUQA number of function values = 173 F = -27274.37754610942 Tog 1.6848935 1.0025849 1.0874118 1.1585570 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF converged at iteration 41 Final energy = -27274.37754610942 SCF con	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.3718664E-01 -3.3766148E-01 .1034051E-02 -6.2243418E-01 -3.3766148E-01 .652411E-01 -4.797497E-01 .20741395-01 .652411E-01 -7.97497E-01 .233230E-01 .2574109E-00 -7.89239E-01 -2.33230E-01 .26179744E-01 .2686146E-02 -1.0499887E-02 .6052348E-02 -3.3602641E-02 -1.0499887E-02 .7912344E-01 2.836496E-02 -1.049887E-02 .7912344E-01 2.836496E-02 -1.049887E-02 .2962445E-03 -1.5389625E-03 -4.5630116E-04 .9966704E-02 8.7101348E-03 .2628490E-03 .9030766E-02 .34003201E-03
707 708 709 710 712 713 714 715 716 717 719 720 727 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 734 737 741 742 744 745 744	At the return from NEWUOA number of function values = 173 F= -27274.37754610942 1.6848935 1.0025849 1.0874118 1.1585570 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 711 1S+ 2S+ 3S+ 4S+ 716 1S+ 2S+ 3S+ 4S+ 717 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 711 3.39455421E-01 6.460758E-04 2.602802E-03 3.7907496E-03 1 722 2.1181678E-01 1.37696582-05 1.050257E-04 1.185370E-03 5.256412E-03 3 724 7.349994E-01 -2.602802E-04 <th>5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.850582E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2184951E-04 -7.3718664E-01 -3.3766148E-01 .602865E-04 -7.3718664E-01 -3.3766148E-01 .602865E-00 1.0136422E+00 3.4555769E-01 .062865E-00 1.0136423E+00 3.4555769E-01 .2365417E-01 1.2190063E-01 -8.2270513E-02 .6179744E-01 2.6666146E-01 -8.2270513E-02 .6179744E-01 2.6666146E-02 -1.0499887E-02 .712344E-01 -8.035950E-02 -2.46634987E-02 .7912344E-03 -1.64946E-03 -6.6634987E-02 .7912344E-04 -3.5464966E-02 -1.1231440E-03 .9966704E-02 8.1013862E-03 -1.652332E-03 .911235E-02 -3.646496E-02 -5.65332E-03 .9030766E-02 5.6108717E-03<</th>	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .9549947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.850582E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2184951E-04 -7.3718664E-01 -3.3766148E-01 .602865E-04 -7.3718664E-01 -3.3766148E-01 .602865E-00 1.0136422E+00 3.4555769E-01 .062865E-00 1.0136423E+00 3.4555769E-01 .2365417E-01 1.2190063E-01 -8.2270513E-02 .6179744E-01 2.6666146E-01 -8.2270513E-02 .6179744E-01 2.6666146E-02 -1.0499887E-02 .712344E-01 -8.035950E-02 -2.46634987E-02 .7912344E-03 -1.64946E-03 -6.6634987E-02 .7912344E-04 -3.5464966E-02 -1.1231440E-03 .9966704E-02 8.1013862E-03 -1.652332E-03 .911235E-02 -3.646496E-02 -5.65332E-03 .9030766E-02 5.6108717E-03<
707 708 709 710 712 713 714 715 716 715 716 717 722 723 724 725 726 727 728 724 725 726 727 728 724 725 726 727 728 729 731 732 733 734 735 737 738 739 731 732 733 734 735 736 737 738 739 731 732 733 734 735 736 737 738 739 731 732 733 734 735 736 737 738 739 731 732 733 734 735 736 737 732 733 734 735 736 737 732 733 734 735 736 737 732 733 734 735 736 737 732 733 734 735 736 737 737 738 737 737 732 733 734 735 736 737 737 737 737 737 737 737 737 737	At the return from NEWUOA number of function values = 173 F= -27274.37754610942 1.6848935 1.0025849 1.0874118 1.1585570 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 713 15 15+ 25+ 35+ 45+ 716 15+ 25+ 35+ 45+ 717 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 719 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 721 1.1371780E-01 6.466178E-06 -0.807512E-05 -6.1594002E-04 -3.759564E-03 -7 722 1.181678E-01 1.3768658E-05 1.0686157E-04 -1.7636196E-03 3.7907496E-03 -7 724 7.349994E-01 -2.775219E-05 -2.4645038E-04 -3.6690518E-03 -1.3768212E-02 1 725 1.3694267E+00 3.5543146E-05 5.664472E-04 4.8195743E-03 -1.3768212E-01 1 726	55+ 65+ 78+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 2.9549947E-05 2.0217706E-04 7.7763953E-01 2.6084676E-04 -1.8505829E-03 1.9084131E-01 2.938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2618495E-04 -7.371664E-01 -3.3766148E-01 .2618495E-00 -0.31664E-01 -3.3766148E-01 .6528111E-01 4.7977497E-01 2.0741439E-01 .052865E-00 1.0136423E+00 3.4555769E-01 .2336517E-01 1.2190063E-01 4.7160748E-02 .65274109E+00 -7.1892239E-01 2.332330E-01 .6179744E-01 2.66643838E-01 8.2270513E-02 .6165244E-01 2.6644473E-02 -1.049887E-02 .7912344E-01 -8.0359590E-02 -2.4606349E-02 .2191235E-02 -3.664296E0-03 -1.13440E-03 .2966704E-02 8.7101348E-03 2.6576332E-03 .2191235E-02 -3.6464966E-02 -1.131440E-02 .29666704E-02 8.710348E-
707 708 709 710 712 713 714 715 716 715 716 717 722 723 724 722 723 724 725 726 727 728 729 731 732 733 734 735 736 737 738 739 737 738 739 734 735 736 737 734 735 736 737 734 735 736 737 734 735 736 736 737 734 735 736 736 737 734 735 736 737 734 735 736 737 737 738 739 734 735 736 737 737 734 735 736 737 737 737 737 737 734 737 737 734 737 737	At the return from NEWUOA number of function values = 173 F= -27274.37754610942 1.6848935 1.0025849 1.0874118 1.1585570 New parameters are 3.2777475E-02 1.8626263E+00 5.3795715E+00 1.6670872E+00 SCF converged at iteration 41 Final energy = -27274.37754610942 711 1S+ 2S+ 3S+ 4S+ 715 1S+ 2S+ 3S+ 4S+ 716 -4.1678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1 717 1 3.2777475E-02 6.3766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8 720 6.1052208E-02 -2.27212503E-06 -2.4851140E-05 2.5997072E-04 1.3479564E-03 -7 721 2.1181678E-01 -1.1776895E-05 -1.0570257E-04 1.1185370E-03 -3.7907496E-03 -1 722 1.13694267E+00 3.5861146E-05 3.5469575E-04 -3.6690519E-03 6.5256712E-03 3 721 1.592004E+00 7.5042538E-05 6.1544024E-04 -6.1554008E-01 -1.5840388E-01 -1 722 1.3694267E+0	5S+ 6S+ 7S+ .1997194E+01 -2.0494257E+00 -1.9849676E-01 .5949947E-05 2.0217706E-04 7.7763953E-01 .6084676E-04 -1.8505829E-03 1.9084131E-01 .5938581E-04 -1.0442761E-02 4.3509449E-01 .2148510E-03 -2.1151300E-01 -4.1956006E-01 .2148510E-03 -2.1151300E-01 -3.3766148E-01 .1094051E-02 -6.2243418E-01 -3.3766148E-01 .652411E-01 .797497E-01 2.0741439E-01 .652411E-01 .797497E-01 -3.3230E-01 .2574109E-00 -7.189239E-01 -8.2270513E-02 .6179744E-01 2.866146E-02 -1.049987E-02 .7912344E-01 -8.0359506E-02 -1.049987E-02 .7912344E-01 -8.0359506E-02 -1.049987E-02 .7912344E-02 -3.602641E-02 -1.049987E-02 .2962445E-03 -1.5389625E-03 -4.5630116E-04 .9030766E-02 -3.46466E-02 -1.1714714E-03 .9030766E-03 -3.01348E-03 1.0152861E-03 .9030766E-03 -3.3103362E-03

750	7.1100931E+08	-2.6913120E-06	-1.1074607E-06	-5.3969183E-07	-2.7956824E-07	-1.3750197E-07	-6.0650654E-08	-1.8595851E-08
751	2.9330971E+09	4.2284342E-07	1.7399041E-07	8.4788201E-08	4.3925941E-08	2.1605380E-08	9.5292259E-09	2.9219333E-09
752	1.3255936E+10	-6.6036810E-08	-2.7172566E-08	-1.3241564E-08	-6.8602231E-09	-3.3743106E-09	-1.4882350E-09	-4.5634558E-10
753	6.5852665E+10	8.2684455E-09	3.4022696E-09	1.6579716E-09	8.5897268E-10	4.2250091E-10	1.8634247E-10	5.7139514E-11
754								
755	2 077747FF 00	6 65020105 00	E 1007121E 00	0 00004005 00	1 40010205 07	1 17007205 07	0 00570705 07	0 0072711E 04
757	6 10E0000E-00	-0.7024960E-09	-2 2024902E-09	-9.0280402E-08	-0 207E010E-07	-1.1702732E-07	-2.2251912E-01	0.09/3/11E-04
758	1 1371780E-01	6 5584587E-08	1 1357878E-07	-1 4021476E-06	2 7503848E-06	-1 7436024E-06	-2.0301400E-00	2.9801280E-04
750	2 1181678E-01	-1 2687135E-07	-2 0131507E-07	3 5750657E-06	-6 7804012E-06	3 7545795E-06	-6 1508803E-03	-1 2202708E-03
760	3 9/55/218-01	2 2202000E-07	6 4801348E-07	-7 5181250E-06	1 /716310E-05	-8 /81/051E-07	-2 9266569E-03	-1 4022390E-03
761	7.3499994E-01	-3.7623323E-07	-1.3240078E-06	1.4888317E-05	-2.7928998E-05	1 1483385E-04	-3.3719703E-03	-1.8292450E-03
762	1.3694267E+00	6.2820434E-07	2.6019932E-06	-2.8314609E-05	4.7559797E-05	2.7010967E-03	3.5481729E-03	1.5339608E-03
763	2.5522453E+00	-1.0548532E-06	-5.1099838E-06	5.0406770E-05	-1.3805043E-04	1.0733461E-02	1.0233838E-02	3 4886688E-03
764	4.7592004E+00	1.7607038E-06	9.3408006E-06	-9.4370031E-05	-2.1881955E-03	1.6938343E-03	1.6747161E-03	6.4816516E-04
765	8.8821010E+00	-2.9467977E-06	-1.6757433E-05	2.1620569E-04	-1.7304956E-02	-2.3680505E-02	-1.3537694E-02	-4.3935092E-03
766	1.6598538E+01	5.1797725E-06	3.8010920E-05	2.0360874E-03	-1.4680955E-02	-1.3203591E-02	-6.8396882E-03	-2.1117539E-03
767	3.1079528E+01	-8.5036007E-06	-7.3720904E-05	2.1595179E-02	3.0642804E-02	1.9816957E-02	9.4758500E-03	2.9149436E-03
768	5.8358006E+01	1.1461839E-05	-1.1455299E-03	3.3856539E-02	3.7345896E-02	2.2720121E-02	1.0478503E-02	3.2554645E-03
769	1.1000966E+02	-2.0387677E-05	-1.7093763E-02	-1.4384488E-02	-9.6242069E-03	-5.1671769E-03	-2.2851648E-03	-7.1377344E-04
770	2.0848751E+02	8.9042294E-05	-4.7607546E-02	-4.9636309E-02	-3.1268197E-02	-1.6208787E-02	-7.2705507E-03	-2.2261834E-03
771	3.9793692E+02	3.1750790E-03	-4.0355126E-02	-3.2905184E-02	-1.9582457E-02	-1.0005800E-02	-4.4379426E-03	-1.3669924E-03
772	7.6660359E+02	2.4905109E-02	2.4571143E-03	-6.4702145E-04	-5.6630997E-04	-3.0559609E-04	-1.4848940E-04	-4.2804830E-05
773	1.4944323E+03	6.4312504E-02	3.5404032E-02	1.8368843E-02	9.6269446E-03	4.7461617E-03	2.1018145E-03	6.4257151E-04
774	2.9570622E+03	8.9937328E-02	4.5939928E-02	2.3407135E-02	1.2284219E-02	6.0646469E-03	2.6744338E-03	8.2093827E-04
775	5.9602824E+03	8.9537818E-02	4.1711583E-02	2.0842689E-02	1.0849360E-02	5.3416257E-03	2.3596508E-03	7.2272164E-04
776	1.2287274E+04	7.3753937E-02	3.2516176E-02	1.6061406E-02	8.3530855E-03	4.1130977E-03	1.8140569E-03	5.5641213E-04
777	2.6025475E+04	5.4420421E-02	2.3238701E-02	1.1407274E-02	5.9138670E-03	2.9087461E-03	1.2840890E-03	3.9342287E-04
778	5.6920168E+04	3.7450532E-02	1.5729658E-02	7.6951575E-03	3.9906895E-03	1.9634095E-03	8.6601592E-04	2.6555365E-04
779	1.2924147E+05	2.4513497E-02	1.0196669E-02	4.9/94708E-03	2.5/87438E-03	1.2680510E-03	5.5964584E-04	1./149460E-04
780	3.0640048E+05	1.5383160E-02	6.36/9065E-03	3.1066330E-03	1.6096318E-03	1.91/1441E-04	3.4923746E-04	1.0/0/400E-04
181	1.629/421E+05	9.2503621E-03	3.81/0961E-03	1.8012148E-03	9.030465/E-04	4./383/92E-04	∠.09098/8E-04	0.4081524E-05
782	2.0076699E+06	5.2989334E-03	2.1831696E-03	1.0641632E-03	5.5118940E-04	2./10/8/6E-04	1.1958448E-04	3.6660831E-05
783	5.0104420E+00	2.8243198E-03	1.1621686E-03	5.6638269E-04	2.9323102E-04	1.4418577E-04	6.3623385E-05	1.9499446E-05
705	1.0002000E+07	1.3403351E-03	5.51195/4E-04	2.0000/00E-04	1.3909661E-04	0.0400047E-05	3.01//964E-05	9.2513066E-06
786	1 88094/5E+08	9.871/00E-04	1.7477703E-04	1 0806300E-06	1 03/3600E-06	5.095/2/8E-07	2 2422000E-07	2.9310403E-00
787	7 1100931E+08	1 162/003E-06	4.00000000E 00	2 3006947E-07	1 175671/E-07	5 7473477E-08	2.2422333E 01	7 7603109E-00
788	2 9330971F+09	-5 6493630E-07	-2 3038071F-07	-1 1220197E-07	-5 7527294F-08	-2 8164677E-08	-1 2508763E-08	-3 8077421F-09
789	1 3255936F+10	2 0123625E-07	8 2100500F-08	3 9986755F-08	2 0510704F-08	1 0043772F-08	4 4594273E-09	1 3578940F-09
790	6.5852665E+10	-5.6896317E-08	-2.3214553E-08	-1.1306646E-08	-5.8000751E-09	-2.8403099E-09	-1.2610270E-09	-3.8400415E-10
791	010002000210	0100000112 00	2102110002 00	11100001012 00	0100001012 00	2101000002 00	1120102102 00	0.01001102 10
792								
793		2P-	3P-	4P-	5P-	6P-		
794		-7.5278343E+02	-1.8645827E+02	-4.6167441E+01	-9.6054318E+00	-1.2842044E+00		
795								
796								
797	3.2777475E-02	-7.1419616E-07	7.8103090E-06	8.0014713E-05	4.1421115E-05	-3.0036559E-04		
798	6.1052208E-02	2.7478595E-06	-2.9964405E-05	-3.0698594E-04	-2.0084087E-04	-4.6908852E-03		
799	1.1371780E-01	-6.1266438E-06	6.6795018E-05	6.7484733E-04	3.4852567E-04	-2.5326033E-02		
800	2.1181678E-01	1.0806498E-05	-1.1735248E-04	-1.1748191E-03	-7.1990125E-04	-1.9859318E-01		
801	3.9455421E-01	-1.7050462E-05	1.8367136E-04	1.8136919E-03	2.4591053E-03	-5.0663001E-01		
802	7.3499994E-01	2.5467950E-05	-2.7268255E-04	-2.5270870E-03	1.8786243E-02	-4.8412064E-01		
803	1.3694267E+00	-3.5833116E-05	4.0248005E-04	3.3854562E-03	2.2862081E-01	5.3893134E-02		
804	2.5522453E+00	5./6655/4E-05	-4.8877642E-04	-7.5621053E-03	6.5921867E-01	4.7808254E-01		
806	4.7592004E+00	-7.1629360E-05	0.11515/3E-04	-/.00000022E-02	4.1932271E-01	2.7962063E-01		
807	1 65985385+01	-2 6568400E-04	-3 2082164E-02	-6 1/26897E-01	-5 0/07795E-01	-2 3595179E-01		
808	3 1079528F+01	3 3486473E-04	-2 6807434F-01	3 5412768E-02	-1 9851858F-02	-1 1221864F-02		
809	5.8358006E+01	6.0909364E-03	-5.3331952E-01	4.5960941E-01	2.4801552E-01	1.0435215E-01		
810	1.1000966E+02	8.1427606E-02	-2.9005669E-01	2.4006230E-01	1.2924157E-01	5.4795638E-02		
811	2.0848751E+02	2.4884351E-01	6.9516352E-02	-2.1149330E-02	-8.3830283E-03	-3.3844827E-03		
812	3.9793692E+02	3.2142412E-01	1.8355468E-01	-9.7197522E-02	-4.6461116E-02	-1.9084088E-02		
813	7.6660359E+02	2.4991232E-01	1.4391088E-01	-7.6545227E-02	-3.6856495E-02	-1.5215454E-02		
814	1.4944323E+03	1.4966669E-01	8.3245213E-02	-4.3851270E-02	-2.0984900E-02	-8.6331107E-03		
815	2.9570622E+03	7.9577568E-02	4.3190468E-02	-2.2617427E-02	-1.0837131E-02	-4.4669823E-03		
816	5.9602824E+03	4.1165686E-02	2.1906788E-02	-1.1412507E-02	-5.4487875E-03	-2.2411963E-03		
817	1.2287274E+04	2.1/64771E-02	1.1463227E-02	-5.9575944E-03	-2.8476002E-03	-1.1/27872E-03		
818	2.60254/5E+04	1.1962129E-02	6.2485980E-03	-3.2404186E-03	-1.5460261E-03	-6.3599606E-04		
819	5.6920168E+04	6.8009560E-03	3.5390295E-03	-1.8337079E-03	-8.7543173E-04	-3.6036597E-04		
821	3 0640048E+05	2 20551/0E-03	2.04/2/03E-03	-1.0599356E-03	-5.0564610E-04	-2.0604375E-04		
822	7 6297/21E+05	1 3185566E-03	6 8270858E-04	-3 5328364E-04	-1 6853580E-04	-6 93/8191E-05		
823	2.0076699E+06	7.3321294E-04	3.7951322E-04	-1.9637484E-04	-9.3691920E-05	-3.8555676E-05		
824	5 010110000000		4 00544405 04	-1 0322601E-04	-4.9245293E-05	-2 02637/1E-05		
825	5.61644261.+06	3.8556276E-04	1.99511488-04	1.03220311.04		2.02037411.0.1		
	1.6802886E+07	3.8556276E-04 1.7968610E-04	9.2969270E-05	-4.8101095E-05	-2.2948263E-05	-9.4433293E-06		
826	5.6164426E+06 1.6802886E+07 5.4065393E+07	3.8556276E-04 1.7968610E-04 5.8601596E-05	9.2969270E-05 3.0318645E-05	-4.8101095E-05 -1.5686187E-05	-2.2948263E-05 -7.4832266E-06	-9.4433293E-06 -3.0792590E-06		
826 827	5.6164426E+06 1.6802886E+07 5.4065393E+07	3.8556276E-04 1.7968610E-04 5.8601596E-05	9.2969270E-05 3.0318645E-05	-4.8101095E-05 -1.5686187E-05	-2.2948263E-05 -7.4832266E-06	-9.4433293E-06 -3.0792590E-06		
826 827 828	5.6164426E+06 1.6802886E+07 5.4065393E+07	3.8556276E-04 1.7968610E-04 5.8601596E-05	9.2969270E-05 3.0318645E-05	-4.8101095E-05 -1.5686187E-05	-2.2948263E-05 -7.4832266E-06	-9.4433293E-06 -3.0792590E-06		
826 827 828 829	3.2777475E-02	3.8556276E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06	1.9951148E-04 9.2969270E-05 3.0318645E-05 7.0000665E-08	-4.8101095E-05 -1.5686187E-05 1.7578676E-06	-2.2948263E-05 -7.4832266E-06 2.5432750E-07	-9.4433293E-06 -3.0792590E-06 -2.2427559E-07		
826 827 828 829 830	3.2777475E-02 6.1052208E-02	3.8556276E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06	1.9951148-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07	-4.8101095E-05 -1.5686187E-05 1.7578676E-06 -1.4049180E-06	-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07	-2.2427559E-07 -9.5509282E-06		
826 827 828 829 830 831	5.6164426E+06 1.6802886E+07 5.4065393E+07 3.2777475E-02 6.1052208E-02 1.1371780E-01	3.85562/6E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06 -1.5158182E-05	1.9951148E-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 3.0331219E-07	-4.8101095E-05 -1.5686187E-05 1.7578676E-06 -1.4049180E-06 4.4901492E-06	-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06	-2.2427559E-07 -9.5509282E-06 -6.9349211E-05		
826 827 828 829 830 831 832	5.6164420E+06 1.6802886E+07 5.4065393E+07 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01	3.8556276E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06 -1.5158182E-05 -4.2451680E-06	1.9951148E-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 3.0331219E-07 -4.7050070E-07	-4.810109E-05 -1.5686187E-05 1.7578676E-06 -1.4049180E-06 4.4901492E-06 -3.5964861E-06	2.248263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06 -2.5070434E-06	-2.2427559E-07 -9.453292E-06 -2.2427559E-07 -9.5509282E-06 -6.9349211E-05 -7.4556346E-04		
826 827 828 829 830 831 832 833	5.6164426E+06 1.6802886E+07 5.4065393E+07 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01	3.8556276E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06 -1.5158182E-05 -4.2451680E-06 -2.2395358E-05	1.951148E-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 3.0331219E-07 -4.7050070E-07 1.1587154E-06	1.05220311 04 -4.8101095E-05 1.5686187E-05 1.7578676E-06 -1.4049180E-06 4.4901492E-06 -3.5964861E-06 1.3135576E-05	2.248263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06 -2.5070434E-06 1.2921192E-05	-2.2427559E-07 -9.5509282E-06 -6.9349211E-05 -7.4556346E-04 -2.5959546E-03		
826 827 828 829 830 831 832 833 833	5.0104426E*00 1.6802386E*07 5.4065393E*07 3.2777475E=02 6.1052208E*02 1.1371780E*01 2.1181678E*01 3.9455421E*01 7.3499994E*01	3.85652/6E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06 -1.5158182E-05 -4.2451680E-06 -2.2395358E-05 -2.4101698E-05	1.9551148E-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 3.0331219E-07 -4.7050070E-07 1.1587154E-06 -1.9000805E-06		-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06 2.5070434E-06 1.2921192E-05 1.3219801E-04	-2.2427559E-07 -9.453293E-06 -3.0792590E-06 -9.5509282E-06 -6.9349211E-05 -7.4556346E-04 -2.5959546E-03 -3.3854786E-03		
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826 827 828 829 830 831 832 833 834 835 836	3.2777475E-02 6.1052208E-07 3.2777475E-02 6.1052208E-02 1.1371780E-01 3.9455421E-01 1.3649297E-00 2.5522453E+00 2.5522453E+00	3.85652/6E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06 -1.5158182E-05 -4.2451680E-06 -2.2395358E-05 -2.4101698E-05 -4.7031223E-05 -6.8311062E-05	1.951148-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 -4.7050070E-07 1.1587154E-06 -1.900805E-06 4.317893E-06 -6.2725455E-06	1.7578676E-06 -1.5686187E-05 1.7578676E-06 -1.4049180E-06 -3.5964861E-06 1.3135576E-05 -1.3264295E-05 -4.0361802E-05 -8.6157072E-05	-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06 -2.5070434E-06 1.3219801E-04 2.1838455E-03 8.5954352E-03	-2.2427559E-07 -9.453293E-06 -3.0792590E-06 -9.5509282E-06 -6.9349211E-05 -7.4556346E-04 -2.5959546E-03 -3.3854786E-03 5.1556783E-04 6.2321848E-03		
826 827 828 829 830 831 832 833 834 835 836 836 837 822	3.2777475E-02 6.1052208E-07 3.2777475E-02 6.1052208E-02 1.1371780E-01 3.9455421E-01 7.349994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00	3.85652/6E-04 1.7968610E-04 5.8601596E-05 5.8601596E-05 4.5611594E-06 -1.5158182E-05 -2.2395358E-05 -2.4101698E-05 -4.7031223E-05 -6.8311062E-05 -1.1523798E-04 1.777540E-05	1.951148-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 4.7050070E-07 1.1587154E-06 -1.9000805E-06 4.3178938E-06 -6.2725455E-06 1.5580022E-05 5.5800727	1.7578676E-06 -1.5686187E-05 1.7578676E-06 -1.4049180E-06 4.4901492E-06 -3.5964861E-06 1.3135576E-05 -1.3264295E-05 -8.6157072E-05 -8.6157072E-05 -1.4997218E-03 1.4857072C	-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06 -2.5070434E-06 1.2921192E-05 1.3219801E-04 2.1838455E-03 8.5954352E-03 7.4633643E-03	-2.2427559E-07 -9.4433293E-06 -3.0792590E-06 -2.2427559E-07 -9.5509282E-06 -6.9349211E-05 -7.4556346E-03 -3.3854786E-03 -3.3854786E-03 5.1556738E-04 6.2321848E-03 4.9748472E-03 4.9748472E-03		
826 827 828 829 830 831 832 833 834 835 836 835 836 837 838 832	5.0104426E*00 1.6802386E*07 5.4065393E*07 6.1052208E*02 1.1371780E*01 3.9455421E*01 7.3499994E*01 1.3694267E*00 2.5522453E*00 4.7592004E*00 8.8821010E*00 8.8821010E*00	3.85652/6E-04 1.7968610E-04 5.8601596E-05 5.8601596E-05 4.5611594E-06 -1.5158182E-05 -2.2395358E-05 -2.4101698E-05 -4.7031223E-05 -6.8311062E-05 -1.1523798E-04 -1.7775408E-04 -2.28582E-04	1.951148-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 3.0331219E-07 -4.7050070E-07 1.1587154E-06 -1.9000805E-06 4.3178993E-06 -6.2725455E-06 1.5580022E-05 -5.3566907E-05	-1.3022031L 0395E-05 -1.5686187E-05 1.7578676E-06 1.4049180E-06 4.4901492E-06 -3.5964861E-06 1.3135576E-05 -1.3264295E-05 4.0361802E-05 -8.6157072E-05 -1.3497218E-03 -1.3851927E-02 -2.2366372E-03	-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06 -2.5070434E-06 1.3291801E-04 2.1383455E-03 3.5954352E-03 7.4633643E-03 -1.0070723E-02 1.6714/98C-02	-2.2427559E-06 -3.0792590E-06 -2.2427559E-07 -9.5509282E-06 -6.9349211E-05 -7.4556346E-04 -2.595546E-03 -3.3854786E-03 5.1556783E-04 6.2321848E-03 4.9748472E-03 -4.615537E-03 -7.7823804E-03		
826 827 828 829 830 831 832 833 834 835 836 837 838 839 840	3.2777475E-02 6.1052208E-07 3.2777475E-02 6.1052208E-02 1.1371780E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00 1.6598538E+01 1.6598538E+01	3.85652/6E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06 -1.5158182E-05 -4.2451680E-06 -2.24951688E-05 -4.7031223E-05 -6.8311062E-05 -1.152378E-04 -1.7775408E-04 -2.9859355E-04 -4.466042E-05	1.951148-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 -4.7050070E-07 1.1587154E-06 4.317893E-06 -6.2725455E-06 -5.3566907E-05 -1.0682392E-03		-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.7480480E-07 1.2252677E-06 -2.5070434E-06 1.3219821-92 1.3219821-92 2.1838455E-03 8.5954352E-03 7.4633643E-03 -1.0070723E-02 -1.6714489E-02 2.837775L72-04	-2.2427559E-06 -3.0792590E-06 -3.0792590E-06 -9.5509282E-06 -6.9349211E-05 -7.4556346E-04 -2.5959546E-03 -3.3854766E-03 5.1556783E-04 6.2321848E-03 -4.6165537E-03 -7.8238944E-03 -4.81902E-04 -4.81902E-04		
826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841	3.2777475E-02 6.1052208E-07 3.2777475E-02 6.1052208E-02 1.1371780E-01 3.9455421E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 1.6598538E+01 3.1079528E+01 3.1079528E+01	3.85652/6E-04 1.7968610E-04 5.8601596E-05 5.8601596E-05 4.2611594E-06 -1.5158182E-05 -4.2451680E-06 -2.2395358E-05 -4.7031223E-05 -6.8311062E-05 -1.7775408E-04 -2.9859355E-04 -4.4960812E-04 -3.6322307E-04	1.951148-04 9.2969270E-05 3.0318645E-05 7.0000665E-08 -1.0155629E-07 -4.7050070E-07 1.1587154E-06 -1.9000805E-06 -4.3178993E-06 -6.2725455E-06 1.5580022E-05 -5.356607E-05 -1.0682392E-03 -1.2235754E-02 -3.328197E-02	1.7578676E-06 -1.4049180E-05 -1.5686187E-05 -1.5686187E-05 -3.5964861E-06 -3.5964861E-06 1.3135576E-05 -1.3264295E-05 -1.3264295E-05 -1.3497218E-03 -1.1851927E-02 -2.0366327E-02 1.7031350E-03 2.8614634E-02	-2.2948263E-05 -7.4832266E-06 2.5432750E-07 -4.740480E-07 1.2252677E-06 -2.5070434E-06 1.3219801E-04 2.1838455E-03 8.5954352E-03 7.4633643E-03 -1.0070723E-02 -1.6714489E-02 -8.3772517E-04	-2.2427559E-07 -9.453293E-06 -3.0792590E-06 -9.5509282E-06 -6.934921E-05 -7.4556346E-04 -2.5959546E-03 -3.3854786E-03 -5.1556783E-04 -6.2321848E-03 4.9748472E-03 -4.6165578-03 -7.8238944E-03 -4.8139265E-04		

842	1.1000966E+02	5.8633180E-03	-2.4755158E-02	2.0357568E-02	1.0947083E-02	4.6403333E-03
843	2.0848751E+02	2.7663532E-02	7.9050943E-03	-2.4590451E-03	-9.8714652E-04	-3.9984555E-04
844	3.9793692E+02	4.9278632E-02	2.8466864E-02	-1.5119849E-02	-7.2324632E-03	-2.9709995E-03
845	7.6660359E+02	5.1169865E-02	2.9666664E-02	-1.5802650E-02	-7.6127992E-03	-3.1434241E-03
846	1.4944323E+03	3.9687448E-02	2.2187704E-02	-1.1701297E-02	-5.5999814E-03	-2.3035144E-03
847	2.9570622E+03	2.6194603E-02	1.4300717E-02	-7.4988679E-03	-3.5955499E-03	-1.4826020E-03
848	5.9602824E+03	1.5931698E-02	8.5328085E-03	-4.4517913E-03	-2.1251481E-03	-8.7380651E-04
849	1.2287274E+04	9.3288421E-03	4.9546810E-03	-2.5802520E-03	-1.2347919E-03	-5.0889786E-04
850	2.6025475E+04	5.3842381E-03	2.8338848E-03	-1.4721886E-03	-7.0212833E-04	-2.8866928E-04
851	5.6920168E+04	3.0926864E-03	1.6225415E-03	-8.4241915E-04	-4.0273993E-04	-1.6592330E-04
852	1.2924147E+05	1.7734094E-03	9.2533153E-04	-4.7969863E-04	-2.2872350E-04	-9.4046964E-05
853	3.0640048E+05	1.0104040E-03	5.2642764E-04	-2.7285039E-04	-1.3034549E-04	-5.3681772E-05
854	7.6297421E+05	5.6708693E-04	2.9446980E-04	-1.5247942E-04	-7.2704287E-05	-2.9900411E-05
855	2.0076699E+06	3.0829826E-04	1.5999996E-04	-8.2847907E-05	-3.9556961E-05	-1.6286587E-05
856	5.6164426E+06	1.5771287E-04	8.1695277E-05	-4.2278166E-05	-2.0160475E-05	-8.2925202E-06
857	1.6802886E+07	7.0609820E-05	3.6575817E-05	-1.8929933E-05	-9.0358362E-06	-3.7196921E-06
858	5.4065393E+07	2.1734831E-05	1.1245924E-05	-5.8182964E-06	-2.7744208E-06	-1.1412212E-06
859						
860						
861		2P+	3P+	4P+	5P+	6P+
862		-6.1939589E+02	-1.5549183E+02	-3.8038164E+01	-7.7221173E+00	-9.5408788E-01
863						
864						
865	3.2777475E-02	-2.4336490E-06	1.6754306E-05	-5.5892525E-05	-6.0387643E-05	1.2386475E-03
866	6.1052208E-02	9.3576855E-06	-6.4207914E-05	2.1493368E-04	3.0280989E-04	1.1874241E-02
867	1.1371780E-01	-2.0842321E-05	1.4278822E-04	-4.6618926E-04	-4.7530162E-04	7.7427164E-02
868	2.1181678E-01	3.6697396E-05	-2.4977203E-04	8.0604051E-04	9.0129034E-04	3.2545555E-01
869	3.9455421E-01	-5.7637303E-05	3.8792609E-04	-1.2273094E-03	-4.6882426E-03	5.3826085E-01
870	7.3499994E-01	8.5352209E-05	-5.6655569E-04	1.5800164E-03	-5.2087664E-02	3.1320799E-01
871	1.3694267E+00	-1.2053399E-04	8.0999454E-04	-1.6846906E-03	-3.6568845E-01	-2.3816734E-01
872	2.5522453E+00	1.7779718E-04	-9.4218169E-04	1.2903151E-02	-6.9361708E-01	-4.5706220E-01
873	4.7592004E+00	-2.2790063E-04	1.3715452E-03	1.6619670E-01	-1.6575956E-01	-1.1313649E-01
874	8.8821010E+00	2.7867735E-04	-4.9912777E-03	6.1780391E-01	5.6618084E-01	2.5261361E-01
875	1.6598538E+01	-5.3063638E-04	-7.6655861E-02	4.7545603E-01	3.7594386E-01	1.6531536E-01
876	3.1079528E+01	8.1926120E-04	-3.9443725E-01	-2.6325439E-01	-1.2640907E-01	-5.0282867E-02
877	5.8358006E+01	1.9516933E-02	-5.3111228E-01	-4.6566357E-01	-2.5019762E-01	-1.0025868E-01
878	1.1000966E+02	1.5033101E-01	-1.3594093E-01	-1.2662521E-01	-6.8504877E-02	-2.7729878E-02
879	2.0848751E+02	3.2133747E-01	1.7641008E-01	9.0446983E-02	4.2739129E-02	1.6796378E-02
880	3.9793692E+02	3.2072249E-01	2.0124520E-01	1.0945733E-01	5.2312345E-02	2.0490470E-02
881	7.6660359E+02	2.0050509E-01	1.2068503E-01	6.4829782E-02	3.0961770E-02	1.2158730E-02
882	1.4944323E+03	9.6326899E-02	5.5757202E-02	2.9651607E-02	1.4096148E-02	5.5177320E-03
883	2.9570622E+03	3.9654466E-02	2.2415263E-02	1.1842862E-02	5.6316919E-03	2.2095082E-03
884	5.9602824E+03	1.4971482E-02	8.3261254E-03	4.3824962E-03	2.0776849E-03	8.1267403E-04
885	1.2287274E+04	5.3674900E-03	2.9641098E-03	1.5566798E-03	7.3927073E-04	2.9002714E-04
886	2.6025475E+04	1.8661840E-03	1.0233010E-03	5.3671985E-04	2.5416668E-04	9.9365917E-05
887	5.6920168E+04	6.3461305E-04	3.4729890E-04	1.8196989E-04	8.6386092E-05	3.3896608E-05
888	1.2924147E+05	2.1249834E-04	1.1571279E-04	6.0588224E-05	2.8673602E-05	1.1205637E-05
889	3.0640048E+05	6.9752539E-05	3.7968687E-05	1.9866465E-05	9.4297765E-06	3.7008695E-06
890	7.6297421E+05	2.2397871E-05	1.2139640E-05	6.3493838E-06	3.0032946E-06	1.1732181E-06
891	2.0076699E+06	6.9131086E-06	3.7504542E-06	1.9605527E-06	9.30/1395E-0/	3.6543963E-07
802	1 6000006E+00	2.0594/01E-06	1.112////E-00	5.0104270E-07	2.7491426E-07	1.0/30215E-0/
804	5 4065393E+07	1 /87078/E-07	2.3073011E 07 8 02//195E-08	1.3000727E 07	1 0700755E-08	7 7181020E-00
895	0110000002-01	1110101012 01	0102111002 00	1110011002 00	1101001002 00	1111010202 00
896						
897	3.2777475E-02	-1.3207878E-09	3.4965780E-08	-7.5446197E-08	-8.3100511E-08	1.8324502E-06
898	6.1052208E-02	1.0946486E-08	-1.6565764E-07	4.0833249E-07	5.8897280E-07	2.3927737E-05
899	1.1371780E-01	-4.0803138E-08	4.7032525E-07	-1.2299178E-06	-1.2621203E-06	2.1304902E-04
900	2.1181678E-01	1.0985682E-07	-1.0728611E-06	2.9362395E-06	3.3058064E-06	1.2220435E-03
901	3.9455421E-01	-2.5276752E-07	2.2024214E-06	-6.1486831E-06	-2.3905280E-05	2.7585314E-03
902	7.3499994E-01	5.3549677E-07	-4.2892502E-06	1.0840453E-05	-3.6457970E-04	2.1905696E-03
903	1.3694267E+00	-1.0650882E-06	8.2210039E-06	-1.5772498E-05	-3.4916695E-03	-2.2739744E-03
904	2.5522453E+00	2.2017354E-06	-1.3001460E-05	1.6782632E-04	-9.0413702E-03	-5.9569861E-03
905	4.7592004E+00	-3.9021382E-06	2.5481600E-05	2.9612675E-03	-2.9460697E-03	-2.0109624E-03
906	8.8821010E+00	6.5774673E-06	-1.2317379E-04	1.5028180E-02	1.3765672E-02	6.1415481E-03
907	1.6598538E+01	-1.7395834E-05	-2.5543939E-03	1.5787682E-02	1.2475252E-02	5.4850895E-03
908	3.1079528E+01	3.7061187E-05	-1.7988429E-02	-1.2006348E-02	-5.7712025E-03	-2.2961420E-03
909	5.8358006E+01	1.2348390E-03	-3.3073785E-02	-2.8932698E-02	-1.5538574E-02	-6.2260449E-03
910	1.1000966E+02	1.3011629E-02	-1.1426030E-02	-1.0640642E-02	-5.7553138E-03	-2.3297340E-03
911	2.0848751E+02	3.8062766E-02	2.0811109E-02	1.0682682E-02	5.0499788E-03	1.9847382E-03
912	3.9793692E+02	5.1851468E-02	3.2230331E-02	1.7496779E-02	8.3583775E-03	3.2735798E-03
913	7.6660359E+02	4.4072294E-02	2.6230738E-02	1.4053605E-02	6.7075174E-03	2.6337808E-03
914	1.4944323E+03	2.8624950E-02	1.6364740E-02	8.6772510E-03	4.1218999E-03	1.6130929E-03
915	2.9570622E+03	1.5770993E-02	8.8005603E-03	4.6349164E-03	2.2024914E-03	8.6408133E-04
916	5.9602824E+03	7.8639115E-03	4.3171518E-03	2.2652863E-03	1.0729240E-03	4.1949616E-04
917	1.2287274E+04	3.6559185E-03	1.9947426E-03	1.0443832E-03	4.9574149E-04	1.9453650E-04
918	2.6025475E+04	1.6113476E-03	8.7355432E-04	4.5694978E-04	2.1613580E-04	8.4425446E-05
919	5.6920168E+04	6.7497388E-04	3.6607705E-04	1.9133996E-04	9.0852090E-05	3.5684824E-05
920	1.2924147E+05	2.6989658E-04	1.4571912E-04	(.6161518E-05	3.5980911E-05	1.4034697E-05
921	3.0640048E+05	1.0215312E-04	5.5349847E-05	2.8914350E-05	1.3745415E-05	5.4085524E-06
922	7.6297421E+05	3.6629771E-05	1.9/32887E-05	1.0312021E-05	4.8624567E-06	1.8917339E-06
923	2.00/6699E+06	1.2254330E-05	0.04//539E-06	3.4/1/529E-06	1.05463/5E-06	0.5339148E-07
924 025	0.0104426E+06	1 0825052E 00	2.0002388E-06	1.0/0/435E-06	1 A7E0204E-07	1.9049028E-U/
920	5 4065303E+07	2 35683868-07	1 2586/0/F-07	6 5813885F_00	3 06426505-00	1 17075/98-09
920	0.4000000E+07	2.000000E-07	1.20004946-07	5.0010000E-08	0.0042000E-00	1.11013405-00
928						
929		3D-	4D-	5D-	6D-	
930		-1.3454927E+02	-2.8439539E+01	-4.0951554E+00	-1.9053474E-01	
931						
932						
933	3.2777475E-02	3.2651074E-07	-2.6571957E-05	-7.1019724E-05	8.9491015E-02	

0.9.4	a 40500000 00	4 40040505 00	0 40400000 05	4 75507000 04	4 00540445 04
934	6.1052208E-02	-1.1894050E-06	9.1843839E-05	1.7552722E-04	1.8654044E-01
935	1.13/1/80E-01	2.4625831E-06	-1.929/146E-04	-5.2234218E-04	3.0652101E-01
936	2.1181678E-01	-4.0986129E-06	3.2129889E-04	-2.7417100E-04	3.2033054E-01
937	3.9455421E-01	6.1043128E-06	-5.0589439E-04	-1.4563385E-02	2.5061410E-01
938	7.3499994E-01	-8.9341665E-06	6.0227820E-04	-1.0696676E-01	8.9685454E-02
939	1.3694267E+00	9.7845165E-06	-7.2930002E-04	-3.4928272E-01	-9.3657675E-02
940	2 5522453E+00	6 1678263E-06	1 2297876E-02	-4 9298781E-01	-1 6224526E-01
0.4.1	4 7592004E+00	-9 5122511E-05	1 23060505-01	-2 2081806E-01	-7 5638/0/E-02
0.4.9	9.0001010E.00	1 7044606E 03	1.2000000E 01	2.2301030E 01	1.0000404E 02
942	0.0021010E+00	-1.7044696E-03	4.0356527E-01	1.9020216E-01	4.00/0442E-02
943	1.6598538E+01	-3.3490722E-02	4.5955502E-01	2.6898485E-01	7.0909914E-02
944	3.1079528E+01	-1.7976659E-01	1.4192470E-01	9.4582711E-02	2.5010988E-02
945	5.8358006E+01	-3.5445132E-01	-1.5547080E-01	-6.1021210E-02	-1.5051975E-02
946	1.1000966E+02	-3.3068223E-01	-1.8988192E-01	-8.3626235E-02	-2.1126171E-02
947	2.0848751E+02	-1.9048277E-01	-1.1074452E-01	-4.8575649E-02	-1.2239840E-02
948	3.9793692E+02	-8.1562455E-02	-4.7076496E-02	-2.0731398E-02	-5.2359922E-03
949	7.6660359E+02	-2.9130071E-02	-1.6474611E-02	-7.1776740E-03	-1.8063717E-03
950	1,4944323E+03	-9.6393649E-03	-5.4487794E-03	-2.3916031E-03	-6.0404305E-04
951	2 9570622F+03	-3 0667014E-03	-1 7080815E-03	-7 4001605E-04	-1 8594553E-04
052	E 0600004E+02	-1 0114007E-02	-E 6907402E-04	-0 40647006-04	-6 2002107E-0E
052	1 0007074E+04	-2 E0204E0E-04	-1 0/9/670E-04	_0 /121026E_0E	-0.1116E16E-0E
054	0.60054755104	1 010202450E 04	6 7021140E 0F	0.4151250E 05	Z.1110310E 03
054	2.0023473E+04	-1.2123034E-04	-0.7931142E-05	-2.9000009E-00	-7.5513092E-00
955	5.6920168E+04	-5.1206264E-05	-2.8281789E-05	-1.22181/2E-05	-3.06/8055E-06
956	1.2924147E+05	-1.2423186E-05	-6.9580184E-06	-3.0604736E-06	-7.7428947E-07
957	3.0640048E+05	-1.0166505E-05	-5.6313512E-06	-2.4435258E-06	-6.1470251E-07
958					
959					
960	3.2777475E-02	5.1272654E-08	-7.1337975E-08	-9.8695082E-08	1.5640040E-04
961	6.1052208E-02	9.4368734E-09	1.9756252E-07	4.1408779E-07	4.4494135E-04
962	1.1371780E-01	1.5149148E-07	-6.8163196E-07	-1.6165852E-06	9.9782587E-04
963	2.1181678E-01	1.7093311E-07	1.2680016E-06	-1.1699505E-06	1.4231482E-03
064	3 9/55/01 01	5 835/0/150-07	-3 3044303E-00	-8 8017777E_05	1 51060975-02
065	7 3/0000/E-01	0 50865765-07	A 2711004E-00	-8 8/076055-04	7 /0135/05-04
900	1.3499994E-01	3.52005/0E-0/	4.2/11904E-06	-0.049/025E-04	1.42130498-04
966	1.3694267E+00	∠.5013533E-06	-9.4/34/02E-06	-3.944/915E-03	-1.05/9134E-03
967	2.5522453E+00	5.1356596E-06	1.8658384E-04	-1.6009953E-03	-2.5015174E-03
968	4.7592004E+00	9.4183882E-06	2.5869202E-03	-4.8349100E-03	-1.5912555E-03
969	8.8821010E+00	-2.4846844E-05	1.1600744E-02	5.4711831E-03	1.3487348E-03
970	1.6598538E+01	-1.2668094E-03	1.8043647E-02	1.0560150E-02	2.7838624E-03
971	3.1079528E+01	-9.5791864E-03	7.5931119E-03	5.0588871E-03	1.3376943E-03
972	5.8358006E+01	-2.5906001E-02	-1.1405232E-02	-4.4834319E-03	-1.1062167E-03
973	1.1000966E+02	-3.2939316E-02	-1.8940614E-02	-8.3445574E-03	-2.1081864E-03
974	2.0848751E+02	-2.5687730E-02	-1,4944831E-02	-6.5558307E-03	-1.6518885E-03
975	3 9793692E+02	-1.4730133E-02	-8.5051338E-03	-3.7462797E-03	-9.4625040E-04
976	7 6660359F+02	-6 8893687F-03	-3 8966271E-03	-1 6970918E-03	-4 2702250E-04
077	1 /0//303E+03	-2 8874401E-03	-1 63/3513E-03	-7 1820842E-04	-1 81/8207E-0/
079	1.4944323E+03	-2.0074401E-03	-1.0343513E-03	-7.1020042E-04	-1.0140297E-04
910	2.9570022E+03	-1.0971088E-03	-0.1041945E-04	-2.03/0/10E-04	-0.0204000E-05
979	5.9602824E+03	-4.1131546E-04	-2.3233303E-04	-1.026/240E-04	-2.601/839E-05
980	4 0000000000000000000000000000000000000				
000	1.228/2/4E+04	-1.4526502E-04	-7.9726162E-05	-3.4004690E-05	-8.4885749E-06
981	2.6025475E+04	-1.4526502E-04 -5.3097540E-05	-7.9726162E-05 -3.0262169E-05	-3.4004690E-05 -1.3565060E-05	-8.4885749E-06 -3.4583031E-06
981 982	1.2287274E+04 2.6025475E+04 5.6920168E+04	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06
981 982 983	1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07
981 982 983 984	1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07
981 982 983 984 985	1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07
981 982 983 984 985 986	1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07
981 982 983 984 985 986 987	1.228/274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 3D+	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 4D+	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07
981 982 983 984 985 986 987 988	1.228/274±+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 3D+ -1.2827939E+02	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.2096828E-06	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07 5D+ -3.8101969E+00	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 6D+ -1.8169381E-01
981 982 983 984 985 986 987 988 989	1.228/2/4E+04 2.60226475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 -3D+ -1.2827939E+02	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07 5D+ -3.8101969E+00	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 6D+ -1.8169381E-01
981 982 983 984 985 986 987 988 989 989	1.228/2/4±04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 -3D+ -1.2827939E+02	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 4D+ -2.6928655E+01	-3.4004690E-05 -1.3565062-05 -4.1025363-06 -1.6064965E-06 -6.3118668E-07 -5D+ -3.8101969E+00	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 6D+ -1.8169381E-01
981 982 983 984 985 986 987 988 989 990 991	1.228/2/4E-04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 3D+ -1.2827939E+02 -4.4802587E-07	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 2.4275314E-05	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07 -3.8101969E+00 -7.5317133E-05	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 -1.8169381E-01 -1.0707794E-01
981 982 983 984 985 986 987 988 989 990 991 992	1.228/2/4E-04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05 3.2777475E-02 6.1052208E-02	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 3D+ -1.2827939E+02 -4.4802587E-07 1.6224646F-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 2.4275314E-05 -8.3565772E-05	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07 -3.8101969E+00 -7.5317133E-05 1.6617400E-04	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 6D+ -1.8169381E-01 -1.0707794E-01 -1.937753E-01
981 982 983 984 985 986 987 988 989 990 991 992 993	1.228/2/4E-04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05 3.2777475E-02 6.1052208E-02 1.1371780E-01	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 3D+ -1.2827939E+02 -4.4802587E-07 1.6222464E-06 -3.3669023E-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 2.4275314E-05 -8.3565772E-05 -8.3565772E-05	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07 5D+ -3.8101969E+00 -7.5317133E-05 1.6617400E-04 -5.8806415E-04	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 6D+ -1.8169381E-01 -1.0707794E-01 -1.9937753E-01 -3.199176E-01
981 982 983 984 985 986 987 988 989 990 991 992 993 994	1.228/2/4E-04 2.6025475E-04 5.6920168E+04 1.2924147E+05 3.0640048E+05 3.0640048E+05 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01	-1.4526502E-04 -5.3097540E-05 -6.0357247E-06 -2.7989375E-06 -2.7989375E-06 -1.2827939E+02 -4.4802587E-07 1.6224646E-06 -3.3669023E-06 -3.3669023E-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 2.4275314E-05 -8.3565772E-05 1.7587412E-04 -2.9003014E-04	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07 -5.8101969E+00 -7.5317133E-05 1.6617400E-04 -5.8806415E-04 -7.3087509E-04	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 -1.8169381E-01 -1.0707794E-01 -1.9937753E-01 -3.157057E-01
981 982 983 984 985 986 987 988 989 990 991 992 993 994 905	1.228/2/4E-04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05 3.0640048E+05 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 2.415742FE-01	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 3D+ -1.2827939E+02 -4.4802587E-07 1.6224646E-06 -3.3669023E-06 5.6351388E-06 -8.3286912E-06	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 2.4275314E-05 -8.3565772E-05 1.7587412E-04 -2.9003014E-04 -2.9003014E-04 -2.9003014E-04	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -1.6064965E-06 -6.3118668E-07 -3.8101969E+00 -7.5317133E-05 1.6617400E-04 -5.8806415E-04 -7.3087509E-04 -1.867656F-02	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 6D+ -1.8169381E-01 -1.937753E-01 -3.1991976E-01 -3.1570572E-01 -3.1570572E-01 -3.1570572E-01
981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 906	1.228/2/4E-04 2.6025475E-04 5.6920168E+04 1.2924147E+05 3.0640048E+05 3.0640048E+05 3.2777475E-02 6.1052208E-02 1.1371780E-01 3.455421E-01 3.455421E-01	-1.4526502E-04 -5.3097540E-05 -6.0357247E-06 -2.7989375E-06 -2.7989375E-06 -1.2827939E+02 -4.4802587E-07 1.6224646E-06 -3.3669023E-06 -6.331388E-06 -8.3286912E-06 -1.42929E-07	-7.9726162E-05 -3.0262168E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 2.4275314E-05 -8.3565772E-05 -8.3565772E-05 1.7587412E-04 -2.9003014E-04 4.651002E-04	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -4.1025343E-06 -6.3118668E-07 -5.8101969E+00 -7.5317133E-05 1.6617400E-04 -7.3087509E-04 -1.8676569E-02 -1.250207E-04	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 -1.8169381E-01 -1.0707794E-01 -1.937753E-01 -3.1590572E-01 -3.1570572E-01 -2.3125690E-01 -2.3125690E-02
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981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997	1.228/2/4E-04 2.6025475E-04 5.6920168E+04 1.2924147E+05 3.0640048E+05 3.0640048E+05 3.2777475E-02 6.1052208E-02 1.371780E-01 2.1181678E-01 3.9455421E-01 7.3499994E-01 1.3694267E+00	-1.4526502E-04 -5.3097540E-05 -1.8273467E-05 -6.0357247E-06 -2.7989375E-06 -2.7989375E-06 -1.2827939E+02 -4.4802587E-07 1.6224646E-06 -3.3669023E-06 -8.3286912E-06 -1.1432832E-05 -1.5216574E-05 -2.216574E-05 -2.216574E-05 -1.5216574E-05 -	-7.9726162E-05 -3.0262169E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 2.4275314E-05 -8.3565772E-05 1.7587412E-04 -2.9003014E-04 4.6510025E-04 -5.5581886E-04 4.6523033E-04 4.6523032E-04	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -4.1025343E-06 -6.3118668E-07 -5.8101969E+00 -7.5317133E-05 1.6617400E-04 -5.8806415E-04 -7.3087509E-04 -1.8676569E-02 -1.2503947E-01 -3.7416157E-01	-8.4885749E-06 -3.4583031E-06 -1.0137506E-06 -4.1341700E-07 -1.5620812E-07 6D+ -1.8169381E-01 -1.937753E-01 -3.1991976E-01 -3.1991976E-01 -3.31570572E-01 -3.3152690E-01 -6.3047095E-02 1.0510482E-01
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381 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 997 998 997 998 990 1000 1001 1003 1004 1005 10010 1011 1012 1013 1014 1015 1016 1017 1018 1021 1022 1022 1023 1025	1.228/2/4E-04 2.6025475E-04 5.6920168E+04 1.2924147E+05 3.0640048E+05 3.0640048E+05 3.0640048E+05 3.0640048E+05 3.9455421E-01 3.9455421E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 3.8521012E+00 3.852204E+00 3.852204E+00 1.6598538E+01 3.1079528E+01 1.1000966E+02 2.0848751E+02 3.9560522E+03 3.2577645E+04 5.9602824E+03 3.26777475E+04 5.9602824E+03 3.0640048E+05 3.0640048E+05 3.2777475E-02 6.1052208E+02 1.371780E+01 2.1181678E+01 2.94521E+01 3.94521E+01 3.945221E+01 3.9454521E+01 3.9454521E+01 3.9454521E+01 3.9455421E+01 3.94555421E+01 3.94555421E+01 3.945555421E+01 3.945555421E+01 3.945555421E+01 3.945555421E+01 3.9455555454200000000000000000000000000000	-1.4526502E-04 -5.3097540E-05 -6.0357247E-06 -2.7989375E-06 -2.7989375E-06 -2.7989375E-06 -1.2827939E+02 -4.4802587E-07 1.6224646E-06 -3.3669023E-06 5.6351388E-06 -8.3286912E-06 1.3216574E-05 -6.0920422E-06 1.32416374E-05 -6.0920422E-06 1.32416374E-05 -6.0920422E-06 1.3241037E-04 2.2622365E-03 4.0492708E-02 1.9887657E-01 3.2180831E-01 1.7529852E-01 3.2180831E-01 1.7529852E-02 6.6296509E-03 1.7162680E-03 4.3584798E-04 1.0119312E-04 2.4512440E-05 5.1949414E-06 1.1521615E-06 3.0400933E-07 -2.55112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-07 -2.4505475E-07 -2	-7.9726162E-05 -3.0262168E-05 -9.8440828E-06 -3.5020021E-06 -1.5096828E-06 -1.5096828E-06 -1.5096828E-06 -1.5096828E-06 -2.6928655E+01 -2.6928655E+01 -2.9003014E-04 4.6510025E-04 -5.5581886E-02 -1.4245950E-01 -4.263314E-01 -4.263314E-01 -4.263314E-01 -4.263314E-01 1.726095E-01 1.726095E-01 1.728095E-01 1.2979953E-02 3.7587050E-03 9.5520955E-04 2.4710517E-04 5.350430E-05 1.4120973E-06 2.7463397E-06 6.8995617E-07 1.5808078E-07 1.9775127E-07 5.6940672E-07 -2.8124617E-06 -2.3882166E-06 5.2366233E-06 -2.3887014E-04	-3.4004690E-05 -1.3565060E-05 -4.1025343E-06 -4.1025343E-06 -6.3118668E-07 5D+ -3.8101969E+00 -7.5317133E-05 1.6617400E-04 -5.8806415E-04 -1.8676569E-02 -1.2503947E-01 -4.8552690E-01 -1.8761814E-03 -3.7416157E-01 -2.1406810E-01 2.1406810E-01 2.1406810E-01 2.5889309E-01 7.5275550E-02 -1.275555E-02 -5.6181141E-03 -1.6416421E-03 -4.4092766E-04 -1.0392766E-04 -1.3246921E-07 -6.2498362E-08 -1.3098950E-07 -1.3101004E-06 -3.2547266E-08 -1.1324607E-04 -1.324726E-03 -1.1324607E-04 -1.324726E-03 -1.1324607E-04 -1.324726E-03 -2.259855E-02 -3.226985E-03 -4.246952E-02 -4.26985E-03 -4.246952E-02 -4.26985E-03 -4.246952E-02 -4.26985E-03 -4.24695E-02 -4.26985E-03 -4.24695E-04 -4.24695E-04 -4.25685E-03 -4.24695E-04 -4.24695	-8. 4885749E-06 -3. 4583031E-06 -1. 0137506E-06 -4. 1341700E-07 -1. 5620812E-07 -1. 5620812E-07 -1. 8169381E-01 -1. 8169381E-01 -1. 9937753E-01 -3. 1991976E-01 -3. 1570572E-01 -3. 1570572E-01 -6. 3047095E-02 1. 0510482E-01 1. 0510482E-01 1. 0510482E-01 1. 0510482E-01 1. 0510482E-01 1. 0520584E-02 2. 0168669E-02 1. 065251E-02 2. 0168669E-02 1. 065251E-02 2. 0168669E-03 1. 3760728E-03 4. 3385296E-03 1. 3760728E-03 4. 0398079E-04 1. 66550027E-06 1. 5822968E-06 2. 631049E-07 8. 2241922E-08 1. 4655020E-08 -1. 8714305E-04 -1. 0214533E-03 -1. 4026622E-03 -1. 4026632E-04 -1. 473506E-04 -1. 473506E-04 -1. 473505E-04 -1. 473505E-04

1026	4 7592004E+00	2 7528844E-06	-3 001814/F-03	-3 0/85280F-03	1 27570835-03
1020	4.7592004E+00	2.7520044E-00	-3.0018144E-03	-3.9403209E-03	-1 E0E7720E-02
1027	1 65095205+01	1 E062020E-02	-1 7471E04E-02	1 0170E70E-00	-2 60701EEE_02
1020	1.0590530E+01	1.5963932E-03	-1.7471504E-02	1.01/05/6E-02	-2.60/9155E-03
1029	3.1079528E+01	1.0724050E-02	-5.6943677E-03	4.0295907E-03	-1.0414543E-03
1030	5.8358006E+01	2.6975934E-02	1.2723409E-02	-5.1328540E-03	1.2409059E-03
1031	1.1000966E+02	3.2419769E-02	1.8801788E-02	-8.2428979E-03	2.0278041E-03
1032	2.0848751E+02	2.4114276E-02	1.4046415E-02	-6.1248998E-03	1.5024841E-03
1033	3.9793692E+02	1.3197018E-02	7.6097968E-03	-3.3285423E-03	8.1849208E-04
1034	7.6660359E+02	5.8221774E-03	3.2862557E-03	-1.4212514E-03	3.4805303E-04
1035	1.4944323E+03	2.2707250E-03	1.2839997E-03	-5.6067292E-04	1.3798793E-04
1036	2.9570622E+03	7.8370384E-04	4.3440158E-04	-1.8606588E-04	4.5400882E-05
1037	5.9602824E+03	2.6332078E-04	1.4918807E-04	-6.5774960E-05	1.6268067E-05
1038	1.2287274E+04	7.8488463E-05	4.2535433E-05	-1.7781357E-05	4.2895664E-06
1039	2.6025475E+04	2.4632134E-05	1.4332594E-05	-6.5269824E-06	1.6378398E-06
1040	5.6920168E+04	6.0733526E-06	3 0796907E-06	-1.1747621E-06	2.7012610E-07
1041	1 2924147F+05	1 8431209E-06	1 1573922E-06	-5 7003982F-07	1 4770355E-07
1042	3 0640048E+05	4 3591834F-07	2 0024127E-07	-6 4421032E-08	1 3266370E-08
1043	0100100102.00	1100010012 01	2100211212 01	0111210022 00	1102000102 00
1044					
1045		4F-	5F-		
1046		-1 4283216F+01	-2 9142420F-01		
1047		1.42032105101	2.31424206 01		
1049					
1040	2 077747EE 00	1 07054715 05	1 00051675 00		
1049	3.2///4/5E-02	-1.0/254/1E-05	1.8335167E-03		
1050	6.1052208E-02	3.73/1/56E-05	1.4299458E-02		
1051	1.1371780E-01	-6.5117205E-05	5.1474113E-02		
1052	2.1181678E-01	1.3410944E-04	1.1826153E-01		
1053	3.9455421E-01	-1.5304599E-04	2.0834794E-01		
1054	7.3499994E-01	3.9034287E-04	2.8704100E-01		
1055	1.3694267E+00	1.8711942E-03	3.1098500E-01		
1056	2.5522453E+00	2.9485902E-02	2.3916164E-01		
1057	4.7592004E+00	1.3401088E-01	9.8299863E-02		
1058	8.8821010E+00	2.9018994E-01	-3.8916120E-02		
1059	1.6598538E+01	3.4836741E-01	-9.0866778E-02		
1060	3.1079528E+01	2.6972459E-01	-7.6747815E-02		
1061	5.8358006E+01	1.4163449E-01	-4.1716302E-02		
1062	1.1000966E+02	5.3462215E-02	-1.5589750E-02		
1063	2 0848751F+02	1 6463172E-02	-4 8330990E-03		
1064	3 9793692F+02	4 0383670F-03	-1 1670891E-03		
1065	7 6660359F+02	9 6404242F-04	-2 8455384F-04		
1066	1 /0//303E+03	2 000033/F-0/	-5 9/38911E-05		
1067	1.4944323E+03	2.0990334E-04	-3.9436911E-05		
1069	2.9570022E+03	4.2739109E-03	-1.2950119E-05		
1000	5.9602624E+03	1.00000005-00	-4.3943503E-06		
1009					
1070					
1071	3.2777475E-02	-2.0783188E-08	3.6300411E-06		
1072	6.1052208E-02	9.3085995E-08	3.8674853E-05		
1073	1.1371780E-01	-2.3659580E-07	1.8998293E-04		
1074	2.1181678E-01	6.3262257E-07	5.9574736E-04		
1075	3.9455421E-01	-1.0880802E-06	1.4323838E-03		
1076	7.3499994E-01	3.4104055E-06	2.6933700E-03		
1077	1.3694267E+00	2.3452890E-05	3.9826033E-03		
1078	2.5522453E+00	5.1386501E-04	4.1805895E-03		
1079	4.7592004E+00	3.1956728E-03	2.3449523E-03		
1080	8.8821010E+00	9.4515168E-03	-1.2688828E-03		
1081	1.6598538E+01	1.5493324E-02	-4.0424851E-03		
1082	3.1079528E+01	1.6367583E-02	-4.6582595E-03		
1083	5.8358006E+01	1.1712012E-02	-3.4499746E-03		
1084	1.1000966E+02	6.0012126E-03	-1.7499308E-03		
1085	2.0848751E+02	2.4902691E-03	-7.3123932E-04		
1086	3.9793692E+02	8.0917742E-04	-2.3369431E-04		
1087	7.6660359E+02	2.5236369E-04	-7.4645254E-05		
1088	1.4944323E+03	6.5321088E-05	-1.8336818E-05		
1089	2.9570622E+03				
1000		1.7865583E-05	-5.4973542E-06		
1090	5.9602824E+03	1.7865583E-05 5.2672434E-06	-5.4973542E-06 -1.4302192E-06		
1090	5.9602824E+03	1.7865583E-05 5.2672434E-06	-5.4973542E-06 -1.4302192E-06		
1090 1091 1092	5.9602824E+03	1.7865583E-05 5.2672434E-06	-5.4973542E-06 -1.4302192E-06		
1090 1091 1092 1093	5.9602824E+03	1.7865583E-05 5.2672434E-06 4F+	-5.4973542E-06 -1.4302192E-06 5F+		
1090 1091 1092 1093 1094	5.9602824E+03	1.7865583E-05 5.2672434E-06 4F+ -1.3898700E+01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01		
1090 1091 1092 1093 1094 1095	5.9602824E+03	1.7865583E-05 5.2672434E-06 4F+ -1.3898700E+01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01		
1090 1091 1092 1093 1094 1095 1096	5.9602824E+03	1.7865582E-05 5.2672434E-06 4F+ -1.3898700E+01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01		
1090 1091 1092 1093 1094 1095 1096 1097	5.9602824E+03 3.2777475E-02	1.7865582E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03		
1090 1091 1092 1093 1094 1095 1096 1097 1098	5.9602824E+03 3.2777475E-02 6.1052208E-02	1.7865583E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01	1.786583E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 7.0857124E-05	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.118167R=01	1.7865832-06 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 7.0857124E-05	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455621E-01	1.7865832-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 7.0857124E-05 -1.4708650E-04 1.684262E-04	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349904E-01	1.7865532-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 -1.4708650E-04 1.6844262E-04 4.269706E-04	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.8764129E-01		
1090 1091 1092 1093 1094 1095 1095 1095 1097 1098 1099 1100 1101 1102	5.9602824E+03 3.2777475E-02 6.1052208E-02 2.1131678E-01 3.9455421E-01 7.349994E-01 1.36427E-02	1.7865832-06 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 7.0857124E-05 1.4708650E-04 1.6844262E-04 -4.2699706E-04 -2.1767361E-02	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.8794124E-01 -3.63392E-01		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349994E-01 1.3694267E+00 2.5522457E+00	1.7865832=-06 5.2672434E=-06 4F+ -1.3898700E+01 1.1675980E=-05 -4.1377000E=-05 7.0857124E=-05 -1.470850E=-04 1.6844262E=-04 -4.2699706E=-04 -2.1767351E=-03 3.203908E=-02	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.8794124E-01 -3.063932E-01 -3.063932E-01		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 2.5522453E+00	1.7865533E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 -1.4708650E-04 1.6844262E-04 4.2699706E-04 -2.1767351E-03 -3.203908E-02 1.400568E-01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.879412E-01 -3.0639932E-01 -2.3140727E-01 -3.98962407E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105	5.9602824E+03 3.2777475E-02 6.1052208E-02 2.11371780E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 4.759204E+00 8.982147E+02	1.7865838-06 5.2672434E-06 4F+ -1.3898700E-05 -4.137700E-05 7.0857124E-05 -1.4708650E-04 1.6844262E-04 -2.1767351E-03 -3.203908E-02 -1.4005668E-01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.3794124E-01 -3.0639932E-01 -2.3140727E-01 -8.9645492E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00	1.7865832-06 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 7.0857124E-05 -1.4708650E-04 -6.24262E-04 -2.1767351E-03 3.203908E-02 -1.4005668E-01 -2.9608946E-01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.8794124E-01 -3.0639932E-01 -3.945492E-02 4.2772328E-02 9.01684-02-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107	5.9602824E+03 3.2777475E-02 6.105208E-02 1.1371780E-01 2.1181678E-01 3.3455421E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00 1.6598538E+01 2.6598538E+01	1.7865583E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 -1.4708650E-04 1.6844262E-04 4.2699706E-04 -2.1767351E-03 -3.2039098E-02 -1.4005668E-01 -2.9608946E-01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.8794124E-01 -3.0639932E-01 -2.3140727E-01 -8.9645492E-02 4.2772328E-02 9.016542E-02 7.42040210		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107 1108	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 4.759204E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01 3.1079528E+01	1.7865838-06 5.2672434E-06 4F+ -1.3898700E-01 1.1675980E-05 7.0857124E-05 -1.4708650E-04 1.6844262E-04 -2.1767351E-03 -3.203908E-02 -1.4005668E-01 -3.4809129E-01 -2.4611894E-01 -1.4641894E-01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.3140727E-01 -3.0639932E-01 -2.3140727E-01 -8.9645492E-02 9.0168542E-02 7.4324210E-02 7.4324210E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107 1108 1109	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.4455421E-01 7.3499994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01 5.3358006E+01	1.7865838-06 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 7.0857124E-05 -1.4708650E-04 -2.1767351E-03 -3.2039088E-02 -1.4005668E-01 -2.9608946E-01 -3.4809129E-01 -3.4809129E-01 -3.4809129E-01 -3.4809129E-01 -2.6411894E-01	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.3140727E-01 -3.063932E-01 -3.9645492E-02 4.2772328E-02 9.0168542E-02 7.4324210E-02 3.9659289E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107 1108 1109 1110	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 2.5522453E+00 3.8221012E+00 1.6598538E+01 3.1079528E+01 5.8358006E+01 1.100996E+02	1.7865838-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 -1.4708650E-04 1.6844262E-04 4.2699706E-04 -2.1767351E-03 -3.203908E-02 -1.4005668E-01 -2.9608946E-01 -2.6411894E-01 -1.3656877E-01 -5.0325596E-02	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.8794124E-01 -3.0639932E-01 -2.3794124E-02 4.2772328E-02 9.0168542E-02 7.4324210E-02 3.9659269E-02 1.4467214E-02		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1102 1103 1106 1107 1108 1109 1101	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 1.34955421E-01 7.349994E-01 1.36942675245E+00 4.759204E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01 5.8358006E+02 2.0848751E+02 2.0848751E+02	1.7865838-06 5.2672434E-06 4F+ -1.3898700E-01 1.1675980E-05 -4.1377000E-05 7.0857124E-05 -1.4708650E-04 1.6844262E-04 -2.1767351E-03 -3.2039098E-02 -1.4005688E-01 -2.9608946E-01 -3.4809129E-01 -3.6808712E-01 -5.0325596E-02 -1.4919582E-02	-5.4973542E-06 -1.4302192E-06 -1.4302192E-06 -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -3.5867071E-02 -1.2737380E-01 -2.1546329E-01 -2.3794124E-01 -3.0639932E-01 -2.3140727E-01 -8.9645492E-02 4.2772328E-02 9.0168542E-02 7.4324210E-02 1.4467214E-02 4.3176435E-02 0.3176435E-02		
10990 1091 1092 1093 1094 1095 1096 1097 1098 10991 1090 1101 1102 1103 1104 1105 1106 1107 1108 1109 1111 1112	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01 5.3358006E+01 2.0848751E+02 3.97938922E+02	1.7865533E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377002E-05 -1.4708650E-04 1.6844262E-04 4.2699706E-04 -2.1767351E-03 -3.2039088E-01 -2.9608946E-01 -3.4809129E-01 -1.3656877E-01 -5.0325596E-02 -1.491562E-02 -3.4681534E-03 	-5.4973542E-06 -1.4302192E-06 5F+ -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.3140727E-01 -3.0639932E-01 -2.3140727E-02 9.0168542E-02 7.4324210E-02 3.9659289E-02 1.4467214E-02 4.317643E-03 9.874238E-03 9.874238E-03		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1106 1107 1108 1109 1110 1111 1112 1113	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 1.3694267E+00 2.5522453E+00 4.759204E+00 8.8821010E+00 1.6598538E+01 5.3358006E+01 1.100966E+02 2.0848751E+02 3.9793692E+02 7.6660359E+02 7.660359E+	1.7865533E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 -1.4708650E-04 1.6844262E-04 4.2699706E-04 -2.1767351E-03 -3.203908E-02 -1.4005668E-01 -2.6411894E-01 -1.3656877E-01 -5.0325596E-02 -3.4681534E-03 -7.6780228E-04 -7.678028E-04 -7	-5.4973542E-06 -1.4302192E-06 -1.4302192E-06 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.8794124E-01 -3.0639932E-01 -3.063932E-02 9.0168542E-02 7.4324210E-02 9.0168542E-02 1.4467214E-02 4.3176435E-03 9.8742368E-04 2.2383383E-04 2.83838E-04 2.2383383E-04		
1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1000 1101 1102 1103 1104 1105 1106 1107 1108 1100 1111 1112 1113 1114	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 7.3499994E-01 1.3694267E+00 4.759204E+00 8.8821010E+00 8.6598538E+01 3.1079528E+01 5.358006E+02 2.0848751E+02 3.9793692E+02 7.6660358E+02 1.4944323E+03	1.7865838-06 5.2672434E-06 4F+ -1.3898700E-05 -4.1377000E-05 7.0857124E-05 -1.4708650E-04 1.6844262E-04 -4.2699706E-04 2.1767351E-03 -3.2039098E-02 -1.4005668E-01 -3.4809129E-01 -3.4809129E-01 -5.0325596E-02 -1.4919582E-02 -3.4681534E-03 -7.6780228E-04 -3.866054E-04	-5.4973542E-06 -1.4302192E-06 -1.4302192E-06 -2.6933365E-01 -2.6792931E-03 -1.7785577E-02 -3.5867071E-02 -1.2737380E-01 -2.1546329E-01 -2.3794124E-01 -3.0639932E-01 -2.3140727E-01 -8.9645492E-02 4.2772328E-02 9.0168542E-02 7.4324210E-02 1.4467214E-02 4.3176435E-03 9.8742386E-04 2.238338E-04 3.8326704E-05		
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1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1000 1101 1102 1103 1104 1105 1100 1111 1112 1113 1114 1115 1116	5.9602824E+03 3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 1.3694267E+00 2.5522453E+00 1.5598538E+01 3.1079528E+01 5.8358006E+01 1.100966E+02 2.0848751E+02 3.9793692E+02 7.6660359E+02 7.6660359E+02 3.9570622E+03 5.9602824E+03	1.7865533E-05 5.2672434E-06 4F+ -1.3898700E+01 1.1675980E-05 -4.1377000E-05 -1.4708650E-04 1.6844262E-04 4.2699706E-04 -2.1767351E-03 -3.2039088E-02 -1.4005668E-01 -2.6411894E-01 -1.3656877E-01 -5.0325596E-02 -1.4919582E-02 -3.4681534E-03 -7.6780228E-04 -1.386654E-03 -2.6734026E-05 -5.2648888E-06	-5.4973542E-06 -1.4302192E-06 -1.4302192E-06 -2.6792931E-03 -1.7785577E-02 -5.8567071E-02 -1.2737380E-01 -2.1546329E-01 -2.1546329E-01 -2.3140727E-01 -3.063932E-01 -3.063932E-02 7.4324210E-02 1.4467214E-02 1.4467214E-02 1.376435E-03 9.8742386E-04 2.2383383E-04 3.8326704E-05 1.3970692E-06		

1118	
1119	3.2777475E-02 2.4030104E-08 -5.3099163E-06
1120	6 1052208F-02 -1 1468771F-07 -4 8102747F-05
1121	$1.1271700E_{-01} = 0.2711000E_{-07} = 0.121262EE_{-04}$
1121	1.13/1/80E-01 2.0/13030E-07 -2.1018033E-04
1122	2.11816/8E-01 -/.5061919E-07 -6.416/480E-04
1123	3.9455421E-01 1.1/3684/E-06 -1.4814308E-03
1124	7.3499994E-01 -4.0316229E-06 -2.7020456E-03
1125	1.3694267E+00 -2.7854269E-05 -3.9245322E-03
1126	2.5522453E+00 -5.6048759E-04 -4.0459078E-03
1127	4.7592004E+00 -3.3449889E-03 -2.1394404E-03
1128	8.8821010E+00 -9.6582637E-03 1.3958154E-03
1129	1.6598538E+01 -1.5510672E-02 4.0174278E-03
1130	3.1079528E+01 -1.6082860E-02 4.5249404E-03
1131	5.8358006E+01 -1.1361507E-02 3.2985776E-03
1132	1.1000966E+02 -5.7154982E-03 1.6425083E-03
1133	2.0848751E+02 -2.3118320E-03 6.6885753E-04
1134	3.9793692E+02 -7.2978324E-04 2.0764163E-04
1135	7.6660359E+02 -2.1946679E-04 6.4005928E-05
1136	1 4944323E+03 -5 2827097E-05 1 4546466E-05
1137	2.9570622E+03 -1.4013535E-05 4.2861177E-06
1138	5.9602824E+03 -3.3747959E-06 8.7670867E-07
1139	
1140	
1141	Coloniated energy = -0.70742775461004165+04
1141	
1144	
1143	Difference $(cal - lit) = 1.36E-03$
1144	Relative error $(abs((cal - lit)/lit)) = 4.99E-08$
1145	Basis set for original program
1146	35 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1147	3.2///4/4514072306E-02 1.0d0 1.0d0
1148	6.1052208024089318E-02 1.0d0 1.0d0
1149	1.1371779544172864E-01 1.0d0 1.0d0
1150	2.1181678224305334E-01 1.0d0 1.0d0
1151	3.9455421330447510E-01 1.0d0 1.0d0
1152	7.3499993917294237E-01 1.0d0 1.0d0
1153	1.3694267119018748E+00 1.0d0 1.0d0
1154	2.5522453323068639E+00 1.0d0 1.0d0
1155	4.7592004160127050E+00 1.0d0 1.0d0
1156	8.8821010163462422E+00 1.0d0 1.0d0
1157	1.6598538397889143E+01 1.0d0 1.0d0
1158	3.1079527707765703E+01 1.0d0 1.0d0
1159	5,8358006063602978E+01 1.0d0 1.0d0
1160	1,1000966104096939E+02,1,0d0,1,0d0
1161	2 0848750508658674E+02 1 0d0 1 0d0
1162	3,9793692474094433E+02,1,0d0,1,0d0
1163	7 6660358942891128E+02 1 0d0 1 0d0
1164	1 49443333346681333E+03 1 0d0 1 0d0
1165	2.05706215767475655103 1.040 1.040
1166	
1100	5.9602824302208819E+03 1.0d0 1.0d0
1107	1.2287273922270530E+04 1.0d0 1.0d0
1168	2.6025474503929181E+04 1.0d0 1.0d0
1109	5.692016794900861/E+04 1.0d0 1.0d0
1170	1.2924146561822579E+05 1.0d0 1.0d0
1171	3.0640047899595002E+05 1.0d0 1.0d0
1172	7.6297421342751326E+05 1.0d0 1.0d0
1173	2.0076698631188064E+06 1.0d0 1.0d0
1174	5.6164425941082174E+06 1.0d0 1.0d0
1175	1.6802885560418982E+07 1.0d0 1.0d0
1176	5.4065392869313173E+07 1.0d0 1.0d0
1177	1.8809445122304142E+08 1.0d0 1.0d0
1178	7.1100930633447683E+08 1.0d0 1.0d0
1179	2.9330970963636436E+09 1.0d0 1.0d0
1180	1.3255935848588299E+10 1.0d0 1.0d0
1181	0.585205468615368/E+10 1.0d0 1.0d0
1182	30 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1183	3.2///4/4514072306E-02 1.0d0 1.0d0
1184	6.1052208024089318E-02 1.0d0 1.0d0
1185	1.13/1//9544172864E-01 1.0d0 1.0d0
1186	2.1181678224305334E-01 1.0d0 1.0d0
1187	3.9455421330447510E-01 1.0d0 1.0d0
1188	7.3499993917294237E-01 1.0d0 1.0d0
1189	1.3694267119018748E+00 1.0d0 1.0d0
1190	2.5522453323068639E+00 1.0d0 1.0d0
1191	4.7592004160127050E+00 1.0d0 1.0d0
1192	8.8821010163462422E+00 1.0d0 1.0d0
1193	1.6598538397889143E+01 1.0d0 1.0d0
1194	3.1079527707765703E+01 1.0d0 1.0d0
1195	5.8358006063602978E+01 1.0d0 1.0d0
1196	1.1000966104096939E+02 1.0d0 1.0d0
1197	2.0848750508658674E+02 1.0d0 1.0d0
1198	3.9793692474094433E+02 1.0d0 1.0d0
1199	7.6660358942891128E+02 1.0d0 1.0d0
1200	1.4944323346681333E+03 1.0d0 1.0d0
1201	2.9570621576747585E+03 1.0d0 1.0d0
1202	5.9602824302208819E+03 1.0d0 1.0d0
1203	1.2287273922270530E+04 1 0d0 1 0d0
1203	2 6025474503929181E+04 1 0d0 1 0d0
1205	5 6920167949008617E+04 1 0d0 1 0d0
1200	1 2924146561822579E+05 1 0d0 1 0d0
1207	3 0640047899595002E+05 1 0d0 1 0d0
1201	7 6207/212/2751226F+05 1 0d0 1 0d0
1208 1200	1.0231421342131320ET03 1.000 1.000 2.0076608631188064E+06 1.0d0 1.0d0
1409	2.0010030031100004ET00 1.000 1.000

1910	i i	E 616442E041082174E+06 1 040 1 040
1210		1 6000000000000000000000000000000000000
1211		1.0002005560410962E+07 1.0d0 1.0d0
1212		5.4065392869313173E+07 1.0d0 1.0d0
1213	30	111111111111111111111111111111111111111
1214		3.2777474514072306E-02 1.0d0 1.0d0
1215		6.1052208024089318E-02 1.0d0 1.0d0
1216		1.1371779544172864E-01 1.0d0 1.0d0
1217		2.1181678224305334E-01 1.0d0 1.0d0
1218		3.9455421330447510E-01 1.0d0 1.0d0
1219		7.3499993917294237E-01 1.0d0 1.0d0
1220		1.3694267119018748E+00 1.0d0 1.0d0
1221		2.5522453323068639E+00 1.0d0 1.0d0
1222		4 7592004160127050E+00 1 0d0 1 0d0
1222		8 8821010163462422E+00 1 0d0 1 0d0
1220		1 65985383978891435+01 1 040 1 040
1005		2 10705077077077077077071 1 010 1 010
1220		5.10/952//0//05/05E+01 1.0d0 1.0d0
1220		5.6556006065602978E+01 1.0d0 1.0d0
1227		1.1000966104096939E+02 1.0d0 1.0d0
1228		2.0848750508658674E+02 1.0d0 1.0d0
1229		3.9793692474094433E+02 1.0d0 1.0d0
1230		7.6660358942891128E+02 1.0d0 1.0d0
1231		1.4944323346681333E+03 1.0d0 1.0d0
1232		2.9570621576747585E+03 1.0d0 1.0d0
1233		5.9602824302208819E+03 1.0d0 1.0d0
1234		1.2287273922270530E+04 1.0d0 1.0d0
1235		2.6025474503929181E+04 1.0d0 1.0d0
1236		5.6920167949008617E+04 1.0d0 1.0d0
1237		1.2924146561822579E+05 1.0d0 1.0d0
1238		3.0640047899595002E+05 1.0d0 1.0d0
1239		7.6297421342751326E+05 1.0d0 1.0d0
1240		2 0076698631188064F+06 1 0d0 1 0d0
1240		5 6164/259/108217/F+06 1 0d0 1 0d0
1241		1 6000000000000000000000000000000000000
1242		1.0002000000000000000000000000000000000
1243		5.40653928693131/3E+0/ 1.0d0 1.0d0
1244	25	
1245		3.2777474514072306E-02 1.0d0 1.0d0
1246		6.1052208024089318E-02 1.0d0 1.0d0
1247		1.1371779544172864E-01 1.0d0 1.0d0
1248		2.1181678224305334E-01 1.0d0 1.0d0
1249		3.9455421330447510E-01 1.0d0 1.0d0
1250		7.3499993917294237E-01 1.0d0 1.0d0
1251		1.3694267119018748E+00 1.0d0 1.0d0
1252		2.5522453323068639E+00 1.0d0 1.0d0
1253		4.7592004160127050E+00 1.0d0 1.0d0
1254		8.8821010163462422E+00 1.0d0 1.0d0
1255		1.6598538397889143E+01 1.0d0 1.0d0
1256		3.1079527707765703E+01 1.0d0 1.0d0
1257		5.8358006063602978E+01.1.0d0.1.0d0
1258		1 1000966104096939E+02 1 040 1 040
1250		2 08487505086586745402 1.0d0 1.0d0
1200		2.0702600474004422E+02 1.040 1.040
1200		3.9793092474094433E+02 1.0d0 1.0d0
1201		7.0000350942091120E+02 1.0d0 1.0d0
1202		1.4944323346681333E+03 1.0d0 1.0d0
1203		2.95/06215/6/4/585E+03 1.0d0 1.0d0
1204		5.9602824302208819E+03 1.0d0 1.0d0
1265		1.2287273922270530E+04 1.0d0 1.0d0
1266		2.6025474503929181E+04 1.0d0 1.0d0
1267		5.6920167949008617E+04 1.0d0 1.0d0
1268		1.2924146561822579E+05 1.0d0 1.0d0
1269		3.0640047899595002E+05 1.0d0 1.0d0
1270	25	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1271		3.2777474514072306E-02 1.0d0 1.0d0
1272		6.1052208024089318E-02 1.0d0 1.0d0
1273		1.1371779544172864E-01 1.0d0 1.0d0
1274		2.1181678224305334E-01 1.0d0 1.0d0
1275		3.9455421330447510E-01 1.0d0 1.0d0
1276		7.3499993917294237E-01 1.0d0 1.0d0
1277		1.3694267119018748E+00 1.0d0 1.0d0
1278		2.5522453323068639E+00 1.0d0 1.0d0
1279		4.7592004160127050E+00 1.0d0 1.0d0
1280		8.8821010163462422E+00 1.0d0 1.0d0
1281		1.6598538397889143E+01 1.0d0 1.0d0
1282		3.1079527707765703E+01 1.0d0 1.0d0
1283		5.8358006063602978E+01 1.0d0 1.0d0
1284		1.1000966104096939E+02 1.0d0 1.0d0
1285		2 0848750508658674E+02 1 0d0 1 0d0
1286		3.9793692474094433E+02 1.0d0 1.0d0
1287		7 6660358942891128E+02 1.0d0 1.0d0
12.88		1.4944323346681333E+03 1.0d0 1.0d0
1280		2 9570621576747585E+03 1 0d0 1 0d0
1200		5 960282/3022088198403 1 040 1 040
1201		1 0087073000077650E104 1 040 1 040
1000		1.2201213722210330ET04 1.000 1.000
1292		2.00234/4303323181E+04 1.0d0 1.0d0
1293		0.0520101545000001/ET04 1.000 1.000
1294		1.29241400018225/9E+05 1.000 1.000
1295	~	3.0640047899595002E+05 1.0d0 1.0d0
1296	20	
1297		3.2///4/4514072306E-02 1.0d0 1.0d0
1298		6.1052208024089318E-02 1.0d0 1.0d0
1299		1.13/1//9544172864E-01 1.0d0 1.0d0
1300		2.1181678224305334E-01 1.0d0 1.0d0
1301	l	3.9455421330447510E-01 1.0d0 1.0d0

1302		7.3499993917294237E-01 1.0d0 1.0d0
1303		1.3694267119018748E+00 1.0d0 1.0d0
1304		2.5522453323068639E+00 1.0d0 1.0d0
1305		4.7592004160127050E+00 1.0d0 1.0d0
1306		8.8821010163462422E+00 1.0d0 1.0d0
1307		1.6598538397889143E+01 1.0d0 1.0d0
1308		3.1079527707765703E+01 1.0d0 1.0d0
1309		5.8358006063602978E+01 1.0d0 1.0d0
1310		1.1000966104096939E+02 1.0d0 1.0d0
1311		2.0848750508658674E+02 1.0d0 1.0d0
1312		3.9793692474094433E+02 1.0d0 1.0d0
1313		7.6660358942891128E+02 1.0d0 1.0d0
1314		1.4944323346681333E+03 1.0d0 1.0d0
1315		2.9570621576747585E+03 1.0d0 1.0d0
1316		5.9602824302208819E+03 1.0d0 1.0d0
1317	20	$1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \$
1318		3.2777474514072306E-02 1.0d0 1.0d0
1319		6.1052208024089318E-02 1.0d0 1.0d0
1320		1.1371779544172864E-01 1.0d0 1.0d0
1321		2.1181678224305334E-01 1.0d0 1.0d0
1322		3.9455421330447510E-01 1.0d0 1.0d0
1323		7.3499993917294237E-01 1.0d0 1.0d0
1324		1.3694267119018748E+00 1.0d0 1.0d0
1325		2.5522453323068639E+00 1.0d0 1.0d0
1326		4.7592004160127050E+00 1.0d0 1.0d0
1327		8.8821010163462422E+00 1.0d0 1.0d0
1328		1.6598538397889143E+01 1.0d0 1.0d0
1329		3.1079527707765703E+01 1.0d0 1.0d0
1330		5.8358006063602978E+01 1.0d0 1.0d0
1331		1.1000966104096939E+02 1.0d0 1.0d0
1332		2.0848750508658674E+02 1.0d0 1.0d0
1333		3.9793692474094433E+02 1.0d0 1.0d0
1334		7.6660358942891128E+02 1.0d0 1.0d0
1335		1.4944323346681333E+03 1.0d0 1.0d0
1336		2.9570621576747585E+03 1.0d0 1.0d0

Listing A.4: Output file for Pa basis set optimization calculation.

A.3 Single Point Energy using a predefined Basis Set

This input file will perform a single point energy calculation on protactinium using the basis optimized in Section A.2.

1	91Pa	
2	<pre>\$contrl jobtype='energy' \$er</pre>	ıd
3	<pre>\$nuc znuc=91 nucmdl=3 \$end</pre>	
4	<pre>\$bas nsym=7 bastype='rdin'</pre>	\$end
5	35	
6	3.2777474514072306E-02	
7	6.1052208024089318E-02	
8	1.1371779544172864E-01	
9	2.1181678224305334E-01	
10	3.9455421330447510E-01	
11	7.3499993917294237E-01	
12	1.3694267119018748E+00	
13	2.5522453323068639E+00	
14	4.7592004160127050E+00	
15	8.8821010163462422E+00	
16	1.6598538397889143E+01	
17	3.1079527707765703E+01	
18	5.8358006063602978E+01	
19	1.1000966104096939E+02	
20	2.0848750508658674E+02	
21	3.9793692474094433E+02	
22	7.6660358942891128E+02	
23	1.4944323346681333E+03	
24	2.9570621576747585E+03	
25	5.9602824302208819E+03	
26	1.2287273922270530E+04	
27	2.6025474503929181E+04	
28	5.6920167949008617E+04	
29	1.2924146561822579E+05	
30	3.0640047899595002E+05	
31	7.6297421342751326E+05	
32	2.0076698631188064E+06	
33	5.6164425941082174E+06	
34	1.6802885560418982E+07	
35	5.4065392869313173E+07	
36	1.8809445122304142E+08	
37	7.1100930633447683E+08	
38	2.9330970963636436E+09	
39	1.3255935848588299E+10	
40	6.5852664686153687E+10	

41	20	
41	30	3 0777474514070306E-02
43		6.1052208024089318E-02
44		1 1371779544172864E-01
45		2.1181678224305334E-01
46		3.9455421330447510E-01
47		7.3499993917294237E-01
48		1.3694267119018748E+00
49		2.5522453323068639E+00
50		4.7592004160127050E+00
51		8.8821010163462422E+00
52		1.6598538397889143E+01
53		3.1079527707765703E+01
54		5.8358006063602978E+01
55		1.1000966104096939E+02
50		2.0848750508658674E+02
59		7 66602500409011095+02
50		1 4044202246691222E+02
60		2 9570621576747585F+03
61		5.9602824302208819E±03
62		1.2287273922270530E+04
63		2.6025474503929181E+04
64		5.6920167949008617E+04
65		1.2924146561822579E+05
66		3.0640047899595002E+05
67		7.6297421342751326E+05
68		2.0076698631188064E+06
69		5.6164425941082174E+06
70		1.6802885560418982E+07
71		5.4065392869313173E+07
72	30	
73		3.2777474514072306E-02
74		6.1052208024089318E-02
75		1.1371779544172864E-01
76		2.1181678224305334E-01
70		3.9455421330447510E-01
70		7.3499993917294237E-01
80		2 5522453323068639E+00
81		4 7592004160127050F+00
82		8.8821010163462422E+00
83		1.6598538397889143E+01
84		3.1079527707765703E+01
85		5.8358006063602978E+01
86		1.1000966104096939E+02
87		2.0848750508658674E+02
88		3.9793692474094433E+02
89		7.6660358942891128E+02
90		1.4944323346681333E+03
91		2.9570621576747585E+03
92		5.9602824302208819E+03
93		1.2287273922270530E+04
94		2.6025474503929181E+04
90		1 2024146561822570E+05
90		1.2924140501022579E+05 3.0640047899595002E+05
98		7.6297421342751326E±05
99		2.0076698631188064E±06
100		5.6164425941082174E+06
101		1.6802885560418982E+07
102		5.4065392869313173E+07
103	25	
104		3.2777474514072306E-02
105		6.1052208024089318E-02
106		1.1371779544172864E-01
107		2.1181678224305334E-01
108		3.9455421330447510E-01
110		1 26042671100187485+00
111		1.309420/119010/405+00
$111 \\ 112$		4 7592004160127050F+00
113		8.8821010163462422E±00
114		1.6598538397889143E+01
115		3.1079527707765703E+01
116		5.8358006063602978E+01
117		1.1000966104096939E+02
118		2.0848750508658674E+02
119		3.9793692474094433E+02
120		7.6660358942891128E+02
121		1.4944323346681333E+03
122		2.95/06215/6747585E+03
123 194		5.9002824302208819E+03
125		2.602547450392419191919
126		5.6920167949008617F+04
127		1.2924146561822579E+05
128		3.0640047899595002E+05
129	25	
130		3.2777474514072306E-02
131		6.1052208024089318E-02
132		1.1371779544172864E-01

1.9.9	0 11016700042052245 01
124	2.11010/0224305534E-01
134	3.9455421550447510E-01
135	7.3499993917294237E-01
136	1.3694267119018748E+00
137	2.5522453323068639E+00
138	4.7592004160127050E+00
139	8.8821010163462422E+00
140	1.6598538397889143E+01
141	3.1079527707765703E+01
142	5.8358006063602978E+01
143	1.1000966104096939E+02
144	2.0848750508658674E+02
145	3.9793692474094433E+02
146	7.6660358942891128E+02
147	1.4944323346681333E+03
148	2.9570621576747585E+03
149	5.9602824302208819E+03
150	1.2287273922270530E+04
151	2.6025474503929181E+04
152	5.6920167949008617E+04
153	1,2924146561822579E+05
154	3.0640047899595002E+05
155	20
156	3 2777474514072306F-02
157	6 1052208024089318E-02
158	1 137177054/17286/F=01
150	2 1181678224305334F-01
160	2.1101070224303334E-01
161	7. 2400002017204027E 01
160	1.20040671100187488100
102	1.3094207119010740E+00
103	2.5522453323068639E+00
104	4.7592004160127050E+00
100	8.8821010163462422E+00
100	1.6598538397889143E+01
167	3.10/952//0//65/03E+01
168	5.8358006063602978E+01
169	1.1000966104096939E+02
170	2.0848750508658674E+02
171	3.9793692474094433E+02
172	7.6660358942891128E+02
173	1.4944323346681333E+03
174	2.9570621576747585E+03
175	5.9602824302208819E+03
176	20
177	3.2777474514072306E-02
178	6.1052208024089318E-02
179	1.1371779544172864E-01
180	2.1181678224305334E-01
181	3.9455421330447510E-01
182	7.3499993917294237E-01
183	1.3694267119018748E+00
184	2.5522453323068639E+00
185	4.7592004160127050E+00
186	8.8821010163462422E+00
187	1.6598538397889143E+01
188	3.1079527707765703E+01
189	5.8358006063602978E+01
190	1.1000966104096939E+02
191	2.0848750508658674E+02
192	3.9793692474094433E+02
193	7.6660358942891128E+02
194	1.4944323346681333E+03
195	2.9570621576747585E+03
196	5.9602824302208819E+03
197	<pre>\$econfig nclose=7 5 5 3 3 1 1 nopen=0 0 0 1 1 1 1 nconf=6 \$end</pre>
198	0.0 0.0 0.0 1.0 0.0 0.0 2.0
199	0.0 0.0 0.0 1.0 0.0 1.0 1.0
200	0.0 0.0 0.0 1.0 0.0 2.0 0.0
201	0.0 0.0 0.0 0.0 1.0 0.0 2.0
202	0.0 0.0 0.0 0.0 1.0 1.0 1.0
203	0.0 0.0 0.0 0.0 1.0 2.0 0.0
204	<pre>\$scf maxitr=100 ixtrp=1 dfctr=0.5 \$end</pre>

Listing A.5: Input file for calculating the single point energy of Pa using a predefined basis set.

1 &CONTRL 2 JUBTYPE = energy, 3 C = 137.0359997600000 4 / 5 &NUC 6 ZNUC = 91.0000000000000, , 7 NUCKDL = 3, 8 RNUC = 0.000000000000, , 9 ALPHA = 129305395.1200000 10 / 2 &BAS 12 NSYM = 7, 13 BASTYPE = rdin ,

14	NGROUP =	1
16	&ECONFIG	
17 18	NCLOSE =	7, 5,
19 20		5, 3.
21		3,
22		1, 1,
24 25	NOPEN =	0, 0,
26		0,
28		1, 1,
29 30		1, 1,
31	FREEEL =	1,
32 33	NCONF =	6
34 35	/ nconf = 6	
36	1 0.00 0.00 0.0	0 1.00 0.00 2.00
37 38	3 0.00 0.00 0.0	0 1.00 0.00 1.00 1.00 0.00
39 40	4 0.00 0.00 0.0	0 0.00 1.00 0.00 2.00
41	6 0.00 0.00 0.0	0 0.00 1.00 2.00 0.00
42 43	MAXITR = 1	00,
$\frac{44}{45}$	IXTRP = DFCTR = 0.500000	1,
46	THDLL = 1.0000000	00000001E-005,
47 48	THDSL = 9.9999999 THDSS = 1.0000000	99999995E-008, 00000001E-009
49 50	/ 31560	
51	166068720	
52 53	82680 82680	
$\frac{54}{55}$	221424960 Calculating one ele	ctron integrals
56	Calculating two ele	ctron integrals
57	Starting SCF	
59 60	SCF converged at it	eration 41 Final energy = -27274.37754610942
61		
63	-4.1	15+ 25+ 55+ 45+ 55+ 65+ 75+ 678552E+03 -7.8202739E+02 -1.9970482E+02 -5.2155429E+01 -1.1997194E+01 -2.0494257E+00 -1.9849676E-01
64 65		
66 67	3.2777475E-02 6.3	766410E-07 5.7309076E-06 -6.1014939E-05 1.3503449E-04 -8.9549947E-05 2.0217706E-04 7.7763953E-01
68	1.1371780E-01 6.4	661788E-06 5.8087512E-05 -6.1594002E-04 1.3479564E-03 -7.5938581E-04 -1.0442761E-02 4.3509449E-01
69 70	2.1181678E-01 -1.1 3.9455421E-01 1.8	776869E-05 -1.0570257E-04 1.1185370E-03 -2.4045368E-03 1.2148510E-03 -2.1151300E-01 -4.1956006E-01 769658E-05 1.6866127E-04 -1.7636196E-03 3.7907496E-03 -1.2618495E-04 -7.3718664E-01 -3.5322441E-01
71	7.3499994E-01 -2.7	775219E-05 -2.4890013E-04 2.6020802E-03 -5.2448412E-03 2.1094051E-02 -6.2243418E-01 -3.3766148E-01
73	2.5522453E+00 -5.5	531012E-05 -5.0644472E-04 4.8195743E-03 -1.3768212E-02 1.0628665E+00 1.0136423E+00 3.4555769E-01
74 75	4.7592004E+00 7.5 8.8821010E+00 -9.9	042533E-05 6.7454424E-04 -6.6562007E-03 -1.5840398E-01 1.2336517E-01 1.2190063E-01 4.7160748E-02 650704E-05 -8.8184744E-04 1.1265810E-02 -9.1814825E-01 -1.2574109E+00 -7.1892239E-01 -2.3332330E-01
$\frac{76}{77}$	1.6598538E+01 1.3	971887E-04 1.4607049E-03 7.8898658E-02 -5.7101352E-01 -5.1418558E-01 -2.6643838E-01 -8.2270513E-02
78	5.8358006E+01 1.6	963083E-04 -2.3283094E-02 7.0220007E-01 7.7741233E-01 4.7333116E-01 2.1834120E-01 6.7834903E-02
79 80	1.1000966E+02 -2.3 2.0848751E+02 8.5	821652E-04 -2.5386103E-01 -2.1304165E-01 -1.4183476E-01 -7.6052348E-02 -3.3602641E-02 -1.0499887E-02 338160E-04 -5.1752274E-01 -5.4684268E-01 -3.4531663E-01 -1.7912344E-01 -8.0359590E-02 -2.4606349E-02
81 82	3.9793692E+02 2.2 7 6660359E+02 1 2	723041E-02 -3.2469759E-01 -2.6916770E-01 -1.6072880E-01 -8.2191235E-02 -3.6464966E-02 -1.1231440E-02
83	1.4944323E+03 2.4	681387E-01 1.4585997E-01 7.6029536E-02 3.9881367E-02 1.9666704E-02 8.7101348E-03 2.6628490E-03
84 85	2.9570622E+03 2.5 5.9602824E+03 1.9	643870E-01 1.4221656E-01 7.3229143E-02 3.8524236E-02 1.9030766E-02 8.3940292E-03 2.5765332E-03 274715E-01 9.7608608E-02 4.9362514E-02 2.5773385E-02 1.2700084E-02 5.6108718E-03 1.7187114E-03
86	1.2287274E+04 1.2	229619E-01 5.8398368E-02 2.9197147E-02 1.5227645E-02 7.5035816E-03 3.3103362E-03 1.0152861E-03
88	5.6920168E+04 4.0	420322-02 3.280136E-02 1.024012E-02 8.4013426E-03 4.1082136E-03 1.040231E-03 5.038977E-04 099771E-02 1.7926580E-02 8.8580193E-03 4.6043650E-03 2.2666591E-03 1.0000444E-03 3.0662309E-04
89 90	1.2924147E+05 2.2 3.0640048E+05 1.2	205546E-02 9.7155189E-03 4.7836464E-03 2.4828387E-03 1.2216568E-03 5.3917832E-04 1.6524649E-04 181181E-02 5.2395866E-03 2.5724532E-03 1.3347501E-03 6.5674013E-04 2.8975990E-04 8.8829643E-05
91	7.6297421E+05 6.6	597693E-03 2.8244368E-03 1.3834892E-03 7.1723201E-04 3.5280484E-04 1.5568362E-04 4.7717415E-05
92 93	5.6164426E+06 1.8	566153E-03 7.7288988E-04 3.7740417E-04 1.9551278E-04 9.6154484E-05 4.2426773E-05 1.3004305E-05
94 95	1.6802886E+07 8.8 5.4065393E+07 3.6	408903E-04 3.6609607E-04 1.7860420E-04 9.2513170E-05 4.5497769E-05 2.0073628E-05 6.1532077E-06 372280E-04 1.5003603E-04 7.3149434E-05 3.7880674E-05 1.8628161E-05 8.2191072E-06 2.5192723E-06
96	1.8809445E+08 3.9	084666E-05 1.6088047E-05 7.8407006E-06 4.0605376E-06 1.9968838E-06 8.8097218E-07 2.7005784E-07 0.13100E-06 1.9076828E-07 0.137002784E-07 0.13700284E-07 0.13700284E-0700284E-0700284E-0700284E-0700284E-0700284E-0700284E-0700284E-0700284E-0700284E-0700284E-07000
97 98	2.9330971E+09 4.2	284342E-07 1.7399041E-07 8.4788201E-08 4.3925941E-08 2.1605380E-08 9.5292259E-09 2.9219333E-09
99 100	1.3255936E+10 -6.6 6.5852665E+10 8.2	036810E-08 -2.7172566E-08 -1.3241564E-08 -6.8602231E-09 -3.3743106E-09 -1.4882350E-09 -4.5634558E-10 684455E-09 3.4022696E-09 1.6579716E-09 8.5897268E-10 4.2250091E-10 1.8634247E-10 5.7139514E-11
101		
102	3.2777475E-02 6.6	583018E-09 5.1997131E-09 -9.0280402E-08 1.4001238E-07 -1.1702732E-07 2.2257972E-07 8.8973711E-04
104	6.1052208E-02 -2.7	234862E-08 -3.3234803E-08 4.8543240E-07 -8.3875912E-07 6.1956519E-07 -2.8561455E-06 2.9801286E-04 584587E-08 1 1357878E-07 -1 4901476E-06 2 7503848E-06 -1 7436034E-06 -2 2330833E-05 9 2701339E-04

107	2 1181678F-01	-1 2687135F-07	-2 9131507F-07	3 5750657F-06	-6 7804012F-06	3 7545795F-06	-6 1508893F-04	-1 2202708F-03
	3 9455421F-01	2 2292090F-07	6 4801348F-07	-7 5181259F-06	1 4716319F-05	-8 4814951F-07	-2 9266569E-03	-1 4022390E-03
100	7 2400004E 01	2.22020000 07	1 2040070E 06	1 4000217E 05	0.7000000000000000000000000000000000000	1 14022055 04	2.02000000 00	1 00004505 00
100	7.3499994E-01	-3.7623323E-07	-1.3240078E-06	1.400031/E-05	-2.7920990E-05	1.1403305E-04	-3.3/19/03E-03	-1.62924506-03
109	1.3694267E+00	6.2820434E-07	2.6019932E-06	-2.8314609E-05	4.7559797E-05	2.7010967E-03	3.5481729E-03	1.5339608E-03
110	2.5522453E+00	-1.0548532E-06	-5.1099838E-06	5.0406770E-05	-1.3805043E-04	1.0733461E-02	1.0233838E-02	3.4886688E-03
111	4.7592004E+00	1.7607038E-06	9.3408006E-06	-9.4370031E-05	-2.1881955E-03	1.6938343E-03	1.6747161E-03	6.4816516E-04
112	8.8821010E+00	-2.9467977E-06	-1.6757433E-05	2.1620569E-04	-1.7304956E-02	-2.3680505E-02	-1.3537694E-02	-4.3935092E-03
113	1.6598538E+01	5.1797725E-06	3.8010920E-05	2.0360874E-03	-1,4680955E-02	-1.3203591E-02	-6.8396882E-03	-2.1117539E-03
114	3 1070528E+01	-8 5036007E-06	-7 3720904E-05	2 1505170E-02	3 0642804E-02	1 0816057E-02	9 4758500E-03	2 01/0/36E-03
115	5.1073520E+01	1 1461020E 0E	1 14FEDOOE 00	2.1000170E 02	3.0042004E 02	0.0700101E 02	1 04705000 00	2.3143450E 03
GIL	5.6356006E+01	1.1401039E-05	-1.1455299E-03	3.3050539E-02	3./345696E-02	2.2/20121E-02	1.04/0503E-02	3.2554645E-03
110	1.1000966E+02	-2.038/6//E-05	-1.7093763E-02	-1.4384488E-02	-9.6242069E-03	-5.16/1/69E-03	-2.2851648E-03	-7.1377344E-04
117	2.0848751E+02	8.9042294E-05	-4.7607546E-02	-4.9636309E-02	-3.1268197E-02	-1.6208787E-02	-7.2705507E-03	-2.2261834E-03
118	3.9793692E+02	3.1750790E-03	-4.0355126E-02	-3.2905184E-02	-1.9582457E-02	-1.0005800E-02	-4.4379426E-03	-1.3669924E-03
119	7.6660359E+02	2.4905109E-02	2.4571143E-03	-6.4702145E-04	-5.6630997E-04	-3.0559609E-04	-1.4848940E-04	-4.2804830E-05
120	1.4944323E+03	6.4312504E-02	3.5404032E-02	1.8368843E-02	9.6269446E-03	4.7461617E-03	2.1018145E-03	6.4257151E-04
121	2 9570622F+03	8 9937328F-02	4 5939928F-02	2 3407135F-02	1 2284219E-02	6 0646469F-03	2 6744338F-03	8 2093827F-04
122	5 9602824E+03	8 0537818E-02	A 1711583E-02	2.0842689E-02	1 08/0360E-02	5 3416257E-03	2 3596508E-03	7 2272164E-04
102	1.0007074E+03	7 3753037E 00	4.1711303E 02	2.0042003E 02	0. 2520055E 02	4 1120077E 02	1.0140ECOE 03	F F641012E 04
120	1.220/2/45+04	1.3/5393/E-02	3.25161/6E-02	1.6061406E-02	0.3530655E-03	4.1130977E-03	1.0140509E-03	5.56412136-04
124	2.6025475E+04	5.4420421E-02	2.3238701E-02	1.1407274E-02	5.9138670E-03	2.9087461E-03	1.2840890E-03	3.9342287E-04
125	5.6920168E+04	3.7450532E-02	1.5729658E-02	7.6951575E-03	3.9906895E-03	1.9634095E-03	8.6601592E-04	2.6555365E-04
126	1.2924147E+05	2.4513497E-02	1.0196669E-02	4.9794708E-03	2.5787438E-03	1.2680510E-03	5.5964584E-04	1.7149460E-04
127	3.0640048E+05	1.5383160E-02	6.3679065E-03	3.1066330E-03	1.6096318E-03	7.9171441E-04	3.4923746E-04	1.0707400E-04
128	7.6297421E+05	9.2503621E-03	3.8170961E-03	1.8612148E-03	9.6364657E-04	4.7383792E-04	2.0909878E-04	6.4081524E-05
129	2 0076699E+06	5 2989334E-03	2 1831696E-03	1 0641632E-03	5 5118940E-04	2 7107876E-04	1 1958448E-04	3 6660831E-05
130	5 6164426E+06	2 82/3108E-03	1 1621686E-03	5 6638269F-04	2 9323102E-04	1 AA18577E-0A	6 3623385E-05	1 9/99//6E-05
1.9.1	1 6000006E107	1 240225150E 03	E E110E74E 04	0.6050203E 04	1 2000001E 04	C 0406047E 05	0.3023303E 03	0.0512060E.06
100	1.0002000E+07	1.3403351E-03	5.51195/4E-04	2.0000/00E-04	1.3909661E-04	0.0400047E-05	3.01//964E-05	9.2513066E-06
132	5.4065393E+07	4.251//66E-04	1./4///65E-04	0.5103139E-05	4.408/413E-05	∠.10///39E-05	9.505/566E-06	∠.9316483E-06
133	1.8809445E+08	9.8714923E-06	4.0808855E-06	1.9896300E-06	1.0343690E-06	5.0954248E-07	2.2422999E-07	6.8918938E-08
134	7.1100931E+08	1.1624993E-06	4.7251887E-07	2.3006947E-07	1.1756714E-07	5.7473477E-08	2.5582624E-08	7.7693109E-09
135	2.9330971E+09	-5.6493630E-07	-2.3038071E-07	-1.1220197E-07	-5.7527294E-08	-2.8164677E-08	-1.2508763E-08	-3.8077421E-09
136	1.3255936E+10	2.0123625E-07	8.2100500E-08	3.9986755E-08	2.0510704E-08	1.0043772E-08	4.4594273E-09	1.3578940E-09
137	6.5852665E+10	-5.6896317E-08	-2.3214553E-08	-1.1306646E-08	-5.8000751E-09	-2.8403099E-09	-1.2610270E-09	-3.8400415E-10
120	0100020002.10	0100000112 00	2102110002 00	1110000102 00	0100001012 00	2101000002 00	1120102.02.00	0101001102 10
120								
139								
140		2P-	3P-	4P-	5P-	6P-		
141		-7.5278343E+02	-1.8645827E+02	-4.6167441E+01	-9.6054318E+00	-1.2842044E+00		
142								
143								
144	3.2777475E-02	-7.1419616E-07	7.8103090E-06	8.0014713E-05	4.1421115E-05	-3.0036559E-04		
145	6 1052208F-02	2 7478595F-06	-2 9964405E-05	-3 0698594F-04	-2 0084087E-04	-4 6908852F-03		
146	1 1371780E-01	-6 1266438E-06	6 6795018E-05	6 7484733E-04	3 4852567E-04	-2 5326033E-02		
147	0 1101670E_01	1 00064005-05	-1 1725040E-04	-1 17/0101E-02	-7 100010FE-04	_1_00E0210E_01		
140	2.11010/06-01	1.0000490E-05	-1.1735240E-04	-1.1/40191E-03	-7.1990125E-04	-1.9039310E-01		
148	3.9455421E-01	-1.7050462E-05	1.836/136E-04	1.8136919E-03	2.4591053E-03	-5.0663001E-01		
149	7.3499994E-01	2.5467950E-05	-2.7268255E-04	-2.5270870E-03	1.8786243E-02	-4.8412064E-01		
150	1.3694267E+00	-3.5833116E-05	4.0248005E-04	3.3854562E-03	2.2862081E-01	5.3893134E-02		
151	2.5522453E+00	5.7665574E-05	-4.8877642E-04	-7.5621053E-03	6.5921867E-01	4.7808254E-01		
152	4.7592004E+00	-7.1829380E-05	8.1151373E-04	-7.6853322E-02	4.1932271E-01	2.7962063E-01		
153	8.8821010E+00	9.0786449E-05	-2.2127713E-03	-4.8837158E-01	-4.1452975E-01	-1.8996887E-01		
154	1 6598538E+01	-2 6568400E-04	-3 2082164E-02	-6 1426897E-01	-5 0407795E-01	-2 3595179E-01		
155	3 1079528F+01	3 3486473F-04	-2 6807434F-01	3 5412768E-02	-1 9851858F-02	-1 1221864F-02		
156	E 02500065101	6.0000364E 02	E 22210EOE 01	4 E060041E 01	0.400100000 02	1.04250155.01		
157	5.6556000E+01	0.0909304E-03	-5.5551952E-01	4.5900941E-01	2.4001002E-01	1.0435215E-01		
157	1.1000966E+02	8.142/606E-02	-2.9005669E-01	2.4006230E-01	1.2924157E-01	5.4795638E-02		
158	2.0848751E+02	2.4884351E-01	6.9516352E-02	-2.1149330E-02	-8.3830283E-03	-3.3844827E-03		
159	3.9793692E+02	3.2142412E-01	1.8355468E-01	-9.7197522E-02	-4.6461116E-02	-1.9084088E-02		
160	7.6660359E+02		1 //3010885-01	7 05 450075 00	0 00504055 00			
161	1.4944323E+03	2.4991232E-01	1.43310005 01	-7.6545227E-02	-3.6856495E-02	-1.5215454E-02		
162		2.4991232E-01 1.4966669E-01	8.3245213E-02	-7.6545227E-02 -4.3851270E-02	-3.6856495E-02 -2.0984900E-02	-1.5215454E-02 -8.6331107E-03		
163	2.9570622E+03	2.4991232E-01 1.4966669E-01 7.9577568E-02	8.3245213E-02 4.3190468E-02	-7.6545227E-02 -4.3851270E-02 -2.2617427E-02	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03		
T O O	2.9570622E+03 5.9602824E+03	2.4991232E-01 1.4966669E-01 7.9577568E-02 4.1165686E-02	8.3245213E-02 4.3190468E-02 2.1906788E-02	-7.6545227E-02 -4.3851270E-02 -2.2617427E-02 -1.1412507E-02	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4487875E-03	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03		
164	2.9570622E+03 5.9602824E+03 1.2287274E+04	2.4991232E-01 1.4966669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02	8.3245213E-02 4.3190468E-02 2.1906788E-02 1.1463227E-02	-7.6545227E-02 -4.3851270E-02 -2.2617427E-02 -1.1412507E-02 -5.9575944E-03	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4487875E-03 -2.8476002E-03	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -1.1727872E-03		
$164 \\ 165$	2.9570622E+03 5.9602824E+03 1.2287274E+04 2.6025475E+04	2.4991232E-01 1.4966669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02 1.1962129E-02	8.3245213E-02 4.3190468E-02 2.1906788E-02 1.1463227E-02 6.2485980E-03	-7.6545227E-02 -4.3851270E-02 -2.2617427E-02 -1.1412507E-02 -5.9575944E-03 -3.2404186E-03	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4487875E-03 -2.8476002E-03 -1.5460261E-03	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -1.1727872E-03 -6.3599606E-04		
164 165	2.9570622E+03 5.9602824E+03 1.2287274E+04 2.6025475E+04	2.4991232E-01 1.4966669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02 1.1962129E-02 6.8009560E-02	8.3245213E-02 4.3190468E-02 2.1906788E-02 1.1463227E-02 6.2485980E-03 3.539020EE-02	-7.6545227E-02 -4.3851270E-02 -2.2617427E-02 -1.1412507E-02 -5.9575944E-03 -3.2404186E-03	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4487875E-03 -2.8476002E-03 -1.5460261E-03 -8.7543172E-04	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -1.1727872E-03 -6.3599606E-04 -3.6036507E-04		
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$164 \\ 165 \\ 166 \\ 167 \\ 160 \\ 160 \\ 160 \\ 100 $	2.9570622E+03 5.9602824E+03 1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05	2.4991232E-01 1.4966669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02 1.1962129E-02 6.8009560E-03 3.9458576E-03	8.3245213E-02 4.3190468E-02 2.1906788E-02 1.1463227E-02 6.2485980E-03 3.5390295E-03 2.0472703E-03	-7.6545227E-02 -4.3851270E-02 -2.2617427E-02 -1.1412507E-02 -5.9575944E-03 -3.2404186E-03 -1.8337079E-03 -1.0599356E-03 -2.45725	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4487875E-03 -2.8476002E-03 -1.5460261E-03 -8.7543173E-04 -5.0564610E-04 -2.0564610E-04	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -1.1727872E-03 -6.3599606E-04 -3.6036597E-04 -2.0804375E-04		
$164 \\ 165 \\ 166 \\ 167 \\ 168 \\ 167 \\ 168 \\ 100 $	2.9570622E+03 5.9602824E+03 1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05	2.4991232E-01 1.496669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02 1.1962129E-02 6.8009560E-03 3.9458576E-03 2.2955149E-03	1.35100501 8.3245213E-02 4.3190468E-02 2.1906788E-02 1.1463227E-02 6.2485980E-03 3.5390295E-03 2.0472703E-03 1.1896197E-03	-7.6545227E-02 -4.3851270E-02 -2.2617427E-02 -5.9575944E-03 -3.2404186E-03 -1.8337079E-03 -1.0599356E-03 -6.1574652E-04 0-20-20-0	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4487875E-03 -2.8476002E-03 -1.5460261E-03 -8.7543173E-04 -5.0564610E-04 -2.9382355E-04	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -1.1727872E-03 -6.359960E-04 -3.6036597E-04 -2.0804375E-04 -1.2092274E-04		
$164 \\ 165 \\ 166 \\ 167 \\ 168 \\ 169$	2.9570622E+03 5.9602824E+03 1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05 7.6297421E+05	2.4991232E-01 1.496669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02 1.1962129E-02 6.8009560E-03 3.9458576E-03 2.2955149E-03 1.3185566E-03	1.351005101 8.3245213E-02 4.3190468E-02 2.1906788E-02 1.1463227E-02 6.2485980E-03 3.5390295E-03 2.0472703E-03 1.1896197E-03 6.8270858E-04	-1.6545227E-02 -4.3851270E-02 -2.2617427E-02 -1.1412507E-02 -5.9575944E-03 -3.2404186E-03 -1.8337079E-03 -1.0599356E-03 -6.1574652E-04 -3.5328364E-04	-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4437875E-03 -2.8476002E-03 -1.5460261E-03 -8.7543173E-04 -5.0564610E-04 -2.9382355E-04 -1.6853589E-04	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -6.3599606E-04 -3.6036597E-04 -2.0804375E-04 -1.2092274E-04 -6.9348191E-05		
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164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195	2.9570622E+03 5.9602824E+03 1.2287274E+04 2.6025475E+04 5.9920168E+04 1.2924147E+05 3.0640048E+05 7.6297421E+05 2.0076699E+06 5.6164426E+06 1.6802886E+07 5.4065393E+07 3.2777475E-02 6.1052208E+02 1.1371780E+01 2.1181678E+01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00 1.6598538E+01 5.8358006E+01 1.100966E+02 2.0948751E+02 3.9793692E+02 7.6660359E+02 7.6660359E+02 1.494432E+03 2.9570622E+03 5.9602824E+03 5.9602824E+03	2.4991232E-01 1.496669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02 1.1962129E-02 6.8009560E-03 3.9458576E-03 7.3321294E-04 1.3185566E-03 7.3321294E-04 1.7968610E-04 5.8601596E-05 -9.3316637E-06 4.5611594E-06 -1.5158182E-05 -4.2451680E-06 -2.2395358E-05 -2.4101698E-05 -4.7031232E-05 -4.7031232E-05 -6.8311062E-05 -1.1523798E-04 -2.985935E-04 -2.985935E-04 -2.985935E-04 -2.985935E-04 -2.985935E-04 -2.985935E-04 -2.985935E-02 -1.1523798E-04 -2.985935E-02 -1.1523798E-04 -2.985935E-02 -1.1523798E-04 -2.985935E-02 -2.101698E-02 2.7663523E-02 3.9687448E-02 2.6194603E-02 1.5931698E-02 2.6194603E-02 1.5931698E	1. ±310050 8. 3245213E-02 4. 3190468E-02 2. 1906788E-02 1. 1463227E-02 6. 2485980E-03 3. 5390295E-03 2. 0472703E-03 1. 1896197E-03 6. 8270858E-04 3. 7951322E-04 1. 9951148E-04 9. 2969270E-05 3. 0318645E-05 7. 0000665E-08 -1. 0155629E-07 -4. 7050070E-07 1. 1587154E-06 -1. 9000805E-06 4. 3178938E-06 -1. 580022E-05 -5. 3566907E-05 -5. 3566907E-05 -1. 0682392E-03 -1. 2235754E-02 -3. 3281971E-02 -2. 4755158E-02 2. 3281971E-02 2. 246664E-02 2. 2487704E-02 1. 4300717E-02		-3.6856495E-02 -2.0984900E-02 -1.0837131E-02 -5.4487875E-03 -2.8476002E-03 -2.8476002E-03 -2.5432735E-04 -3.6853589E-04 -2.9382355E-04 -2.9382355E-04 -2.9382355E-04 -3.93691920E-05 -4.9245293E-05 -7.4832266E-06 1.2921192E-05 1.3219801E-04 2.138445E-03 8.5954352E-03 7.4633643E-03 -1.6714489E-02 -1.6714489E-02 -1.6714489E-02 -1.6714489E-02 -1.6714489E-02 -3.51595431E-03 -7.2324632E-03 -7.6127992E-03 -5.599814E-03 -5.599814E-03 -5.599814E-03 -5.599814E-03 -5.599814E-03 -5.599814E-03 -5.599814E-03 -5.599814E-03 -5.599814E-03 -3.5555499E-03 -2.1251481E-03 -1.225147E-04 -1.225147E-04 -1.225492E-03 -3.5555499E-03 -2.1251481E-03 -1.225147E-04 -1.225147E-04 -1.225147E-04 -1.225447E-04 -3.5555499E-03 -2.1251481E-03 -1.22547E-04 -1.225492E-03 -2.1251481E-03 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.2554582E-04 -2.25	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -1.1727872E-03 -6.3599606E-04 -3.6036597E-04 -2.0804375E-04 -1.2092274E-04 -1.2092274E-04 -2.2083741E-05 -3.8555676E-05 -9.4433293E-06 -6.9349211E-05 -7.4556346E-04 -2.59559546E-03 -3.3854786E-03 5.1556783E-04 6.2321848E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.3854786E-03 -3.398455E-04 -2.9709995E-03 -3.1434241E-03 -2.3035144E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.30544E-03 -2.3		
$\begin{array}{c} 164\\ 165\\ 166\\ 167\\ 168\\ 169\\ 170\\ 171\\ 172\\ 173\\ 174\\ 175\\ 176\\ 177\\ 178\\ 179\\ 180\\ 181\\ 182\\ 183\\ 184\\ 185\\ 186\\ 187\\ 188\\ 189\\ 190\\ 191\\ 192\\ 193\\ 194\\ 195\\ 196\\ 197\\ \end{array}$	2.9570622E+03 5.9602824E+03 1.2287274E+04 2.6025475E+04 5.6920168E+04 1.2924147E+05 3.0640048E+05 7.6297421E+05 5.0076699E+06 5.6164426E+06 1.6802866E+07 5.4065393E+07 3.2777475E-02 6.1052208E+07 3.9455421E+01 7.349994E+01 1.364267E+00 2.5522453E+00 4.759204E+00 1.6598538E+01 3.1079528E+01 1.1000966E+02 2.0848751E+02 2.9793692E+02 7.6660359E+02 1.4944323E+03 2.9570622E+03 5.9602824E+03 1.2287274E+04	2.4991232E-01 1.496669E-01 7.9577568E-02 4.1165686E-02 2.1764771E-02 1.1962129E-02 6.8009560E-03 3.9458576E-03 2.2955149E-03 1.3185566E-03 1.3185562F-04 1.7968610E-04 3.8566276E-04 1.7968610E-04 4.5611594E-06 -1.5158182E-05 -2.4101698E-05 -2.4395358E-05 -2.4101698E-05 -2.4395358E-05 -2.4101698E-05 -2.4395358E-04 -1.7775408E-04 -2.9859355E-04 -4.9603122E-05 -1.17775408E-04 -2.9859355E-04 -4.9603122E-05 -1.17776408E-04 -2.9859355E-04 -4.9603122E-05 -1.17776408E-04 -2.9859355E-04 -4.960312E-04 -2.9859355E-04 -2.49766352E-02 3.6827448E-02 2.6194603E-02 1.5931698E-02 9.3282421E-03 5.384294E-02 9.3282421E-03 5.384294E-02 9.3282421E-03 5.384294E-02 9.3282421E-03 5.384294E-02 9.3282421E-03 5.384294E-02 9.3282421E-03 5.384294E-02 9.3282421E-03 5.384294284E-03 5.384294E-03 5.384294E-03 5.384294E-03	1. 3245213E-02 4. 3190468E-02 2. 1906788E-02 1. 1463227E-02 6. 2485980E-03 3. 5390295E-03 2. 0472703E-03 1. 1896197E-03 6. 8270858E-04 3. 7951322E-04 1. 9951148E-04 9. 2969270E-05 3. 0318645E-05 7. 0000665E-08 -1. 0155629E-07 3. 0331219E-07 -4. 7050070E-07 1. 1587154E-06 -1. 9000805E-06 -1. 9000805E-06 -5. 3566907E-05 -3. 3281971E-02 -3. 3281971E-02 -3. 3281971E-02 -2. 4755158E-02 7. 9050943E-03 2. 8466864E-02 2. 2187704E-02 2. 14300717E-02 8. 5328085E-03 4. 9546810E-03 2. 8456810E-03 4. 9546810E-03 2. 8456840E-02 2. 8456840E-02 2. 966664E-02 2. 966664E-02 3. 966		-3. 6856495E-02 -2. 0984900E-02 -1. 0837131E-02 -5. 4487875E-03 -1. 5460261E-03 -8. 7543173E-04 -2. 9376002E-03 -8. 7543173E-04 -2. 9382355E-04 -1. 6853589E-04 -1. 6853589E-04 -1. 6853589E-04 -2. 9382355E-05 -2. 2948263E-05 -7. 4832266E-06 2. 5070434E-06 1. 2921192E-05 1. 3219801E-04 2. 1838455E-03 7. 4633643E-03 8. 5954352E-03 7. 4633643E-03 1. 007073E-02 -1. 6714489E-02 -8. 3772517E-04 1. 5437728E-02 -1. 6714489E-02 -8. 3772517E-04 1. 5437728E-02 -7. 2324632E-03 -7. 12792E-03 -3. 5955499E-03 -3. 5955499E-03 -2. 1251481E-03 -1. 1251481E-03 -7. 0212832E-04	-1.5215454E-02 -8.6331107E-03 -4.4669823E-03 -2.2411963E-03 -1.1727872E-03 -6.3559606E-04 -3.6036597E-04 -2.0804375E-04 -6.9348191E-05 -3.8555676E-05 -2.0263741E-05 -9.4433293E-06 -3.0792590E-06 -2.2427559E-07 -6.9349211E-05 -7.4556346E-04 -2.5959546E-03 -3.3854766E-03 -3.3854766E-03 -3.3854766E-03 -3.385476E-03 -3.385476E-03 -4.6165537E-03 -4.8139265E-04 -6.4952597E-03 -4.61955257E-03 -3.984555E-04 -2.579955E-04 -2.373051424E-03 -3.342421E-03 -3.342421E-03 -2.3730551E-04 -2.888976E-04 -5.088976E-04		

198	5 6920168F+04	3 0926864F-03	1 6225415F-03	-8 4241915E-04	-4 0273993F-04	-1 6592330F-04
199	1.2924147E+05	1.7734094E-03	9.2533153E-04	-4.7969863E-04	-2.2872350E-04	-9.4046964E-05
200	3.0640048E+05	1.0104040E-03	5.2642764E-04	-2.7285039E-04	-1.3034549E-04	-5.3681772E-05
201	7.6297421E+05	5.6708693E-04	2.9446980E-04	-1.5247942E-04	-7.2704287E-05	-2.9900411E-05
202	2.0076699E+06	3.0829826E-04	1.5999996E-04	-8.2847907E-05	-3.9556961E-05	-1.6286587E-05
202	5 6164426E+06	1 5771287E-04	8 1695277F-05	-4 2278166E-05	-2 0160475E-05	-8 2925202F-06
204	1.6802886E+07	7.0609820E-05	3.6575817E-05	-1.8929933E-05	-9.0358362E-06	-3.7196921E-06
205	5 4065393E+07	2 1734831F-05	1 1245924F-05	-5 8182964F-06	-2 7744208F-06	-1 1412212E-06
206	0.400000000	2.11040011 00	1.12405241 00	0.01020011 00	2.11442001 00	1.14122120 00
200						
201		20+	30+	1P+	5D+	6P+
209		-6.1939589E+02	-1.5549183E+02	-3.8038164E+01	-7.7221173E+00	-9.5408788E-01
210		0.1000000102	1.00401000002	0.00001041.01	1.12211101.00	5.0400/00E 01
210						
212	3 2777475F-02	-2 4336490F-06	1 6754306F-05	-5 5892525F-05	-6 0387643F-05	1 2386475F-03
213	6 1052208E-02	9 3576855F-06	-6 4207914F-05	2 1493368E-04	3 0280989F-04	1 1874241F-02
210	1 1371780F-01	-2 0842321F-05	1 4278822F-04	-4 6618926E-04	-4 7530162F-04	7 7427164F-02
214	0 1101670E-01	2.0042321E 03	-0 40770022E 04	9.06040E1E-04	9.0100024E-04	2 DEAEEEEE_01
210	3 9455421E-01	-5 7637303E-05	3 8792609E-04	-1 227300/F-03	-4 6882426E-03	5.2040000E 01
210	7 3/0000/F-01	8 5352209E-05	-5 6655569E-04	1 580016/E-03	-4.0882420E-03	3 1320700E-01
218	1 369/267E+00	-1 2053300E-04	8 000000000000000000000000000000000000	-1 68/6906E-03	-3 65688/5E-01	-2 381673/F-01
210	2 5522453E+00	1 7770718E-04	-0 /218160E-04	1 2003151E-02	-5.0508845E-01	-2.3810734E-01
213	2.3322433E+00	-2 2700062E-04	1 27164606-02	1.2303131E 02	-1 65750565-01	-1 1212640E-01
220	4.7592004E+00	2.2790003E-04	-4 0010777E-02	6 1790201E-01	-1.03/3930E-01	-1.1313049E-01
221	1 6E00E20E+01	_E 2062620E_04	-4.9912///E-03	4 7E4E602E-01	2 7E0/206E-01	2.5201301E-01
222	1.0590550E+01	-5.3003036E-04	-7.0055601E-02	4.7545003E-01	1.0640007E 01	1.0001000E-01
223	5.1079526E+01	1 0E16022E-02	-5.9443723E-01	-2.0323439E-01	-1.2040907E-01	-3.0282807E-02
224	1 1000066E+02	1.9510955E-02	-5.3111228E-01	-4.0300337E-01	-2.3019702E-01	-1.0025808E-01
220	1.1000900E+02	2 0122747E-01	1 76410095E-01	-1.2002521E-01	4 0720100E-02	1 6706279E-02
220	2.0040751E+02	3.2133/4/E-01	1.7641006E-01	9.0446963E-02	4.2/39129E-02	1.0/903/0E-02
221	3.9/93092E+02	3.2072249E-01	2.0124520E-01	1.0945755E-01	5.2312345E-02	2.0490470E-02
220	1 4044202E+02	2.0050509E-01	1.2000503E-01	0.4029/02E-02	3.0901//0E-02	1.2156/30E-02
229	1.4944323E+03	3.0320039E-02	0.015/202E-02	2.30310U/E-02	1.4090148E-02	0.01//32UE-03
230	2.9570622E+03	3.9654466E-02	2.2415263E-02	1.1842862E-02	5.6316919E-03	2.2095082E-03
231	5.9602824E+03	1.4971482E-02	8.3261254E-03	4.3824962E-03	2.0776849E-03	8.126/403E-04
232	1.2207274E+04	5.3674900E-03	2.9641096E-03	1.5566/96E-03	7.3927073E-04	2.9002/14E-04
233	2.6025475E+04	1.8661840E-03	1.0233010E-03	5.36/1985E-04	2.5416668E-04	9.9365917E-05
234	5.6920166E+04	6.3461305E-04	3.4729690E-04	1.0196969E-04	0.0306092E-05	3.3090000E-05
230	1.2924147E+05	2.1249834E-04	1.15/12/9E-04	6.0588224E-05	2.86/3602E-05	1.1205637E-05
230	3.0640048E+05	6.9752539E-05	3.7968687E-05	1.9866465E-05	9.4297765E-06	3.7008695E-06
201	7.6297421E+05	2.239/0/1E-05	1.2139640E-05	0.3493636E-06	3.0032946E-06	1.1/32101E-00
200	2.0076699E+06	0.9131000E-00	3.7504542E-06	1.9605527E-06	9.30/1395E-07	3.0543903E-07
239	1 6000006E+07	2.0394701E-00	0.097E011E-07	1 E609707E-07	Z.1491420E-01	0.0160E11E-09
240	1.0002000E+07	1 4070704E 07	2.90/3011E-0/	1.3000727E-07	1.4104034E-08	Z.9100311E-08
241	5.4065393E+07	1.40/9/046-0/	0.0244195E-00	4.1931/30E-00	1.9/99/555-06	1.1101920E-09
242						
243	3 07774755-00	-1 3207878F-09	3 49657805-08	-7 5446197E-08	-8 3100511E-08	1 83245025-06
244	6 1052208E-02	1.00/6/86E-08	-1 6565764E-07	/ 08332/0E-07	5 8807280E-07	2 3027737E-05
240	1 1271700E-01	_1.0940400E-00	4 7020E0EE-07	4.0033249E-07	-1 0601200E-01	2.392//3/E-03
240	2 1181678E-01	1 0085682E-07	-1 0728611E-06	-1.2299178E-00	-1.2021203E-00	1 2220435E-03
241	2.1101070E-01	-0 E0767E0E-07	-1.0728011E-00	2.9302393E-00	-2 200E200E_0E	0 7E9E214E-02
240	7 3/0000/F-01	5 35/0677E-07	-4 2892502E-06	1 0840453E-05	-2.3903280E-03	2.7565514E-03
250	1 369/267E+00	-1 0650882E-06	9.2032002E 00	-1 5772/08E-05	-3 /016605E-03	-2 273074/F-03
251	2 5522453E+00	2 2017354E-06	-1 3001/60E-05	1.6782632E-04	-9 0/13702E-03	-5 9569861E-03
252	4 7592004F+00	-3 9021382F-06	2 5481600F-05	2 9612675E-03	-2 9460697E-03	-2 0109624F-03
253	8.8821010E+00	6.5774673E-06	-1.2317379E-04	1.5028180E-02	1.3765672E-02	6.1415481E-03
254	1.6598538E+01	-1.7395834E-05	-2.5543939E-03	1.5787682E-02	1.2475252E-02	5.4850895E-03
255	3.1079528E+01	3.7061187E-05	-1.7988429E-02	-1.2006348E-02	-5.7712025E-03	-2.2961420E-03
256	5.8358006E+01	1.2348390E-03	-3.3073785E-02	-2.8932698E-02	-1.5538574E-02	-6.2260449E-03
257	1.1000966E+02	1.3011629E-02	-1.1426030E-02	-1.0640642E-02	-5.7553138E-03	-2.3297340E-03
258	2.0848751E+02	3.8062766E-02	2.0811109E-02	1.0682682E-02	5.0499788E-03	1.9847382E-03
259	3.9793692E+02	5.1851468E-02	3.2230331E-02	1.7496779E-02	8.3583775E-03	3.2735798E-03
260	7.6660359E+02	4.4072294E-02	2.6230738E-02	1.4053605E-02	6.7075174E-03	2.6337808E-03
261	1.4944323E+03	2.8624950E-02	1.6364740E-02	8.6772510E-03	4.1218999E-03	1.6130929E-03
262	2.9570622E+03	1.5770993E-02	8.8005603E-03	4.6349164E-03	2.2024914E-03	8.6408133E-04
263	5.9602824E+03	7.8639115E-03	4.3171518E-03	2.2652863E-03	1.0729240E-03	4.1949616E-04
264	1.2287274E+04	3.6559185E-03	1.9947426E-03	1.0443832E-03	4.9574149E-04	1.9453650E-04
265	2.6025475E+04	1.6113476E-03	8.7355432E-04	4.5694978E-04	2.1613580E-04	8.4425446E-05
266	5.6920168E+04	6.7497388E-04	3.6607705E-04	1.9133996E-04	9.0852090E-05	3.5684824E-05
267	1.2924147E+05	2.6989658E-04	1.4571912E-04	7.6161518E-05	3.5980911E-05	1.4034697E-05
268	3.0640048E+05	1.0215312E-04	5.5349847E-05	2.8914350E-05	1.3745415E-05	5.4085524E-06
269	7.6297421E+05	3.6629771E-05	1.9732887E-05	1.0312021E-05	4.8624567E-06	1.8917339E-06
270	2.0076699E+06	1.2254330E-05	6.6477539E-06	3.4717529E-06	1.6546375E-06	6.5339148E-07
271	5.6164426E+06	3.8316748E-06	2.0582388E-06	1.0757435E-06	5.0527204E-07	1.9549628E-07
272	1.6802886E+07	1.0835857E-06	5.8992873E-07	3.0797781E-07	1.4759391E-07	5.8723790E-08
273	5.4065393E+07	2.3568386E-07	1.2586494E-07	6.5813885E-08	3.0642650E-08	1.1707548E-08
274						
275						
276		3D-	4D-	5D-	6D-	
277		-1.3454927E+02	-2.8439539E+01	-4.0951554E+00	-1.9053474E-01	
278						
279						
280	3.2777475E-02	3.2651074E-07	-2.6571957E-05	-7.1019724E-05	8.9491015E-02	
281	6.1052208E-02	-1.1894050E-06	9.1843839E-05	1.7552722E-04	1.8654044E-01	
282	1.1371780E-01	2.4625831E-06	-1.9297146E-04	-5.2234218E-04	3.0652101E-01	
283	2.1181678E-01	-4.0986129E-06	3.2129889E-04	-2.7417100E-04	3.2033054E-01	
284	3.9455421E-01	6.1043128E-06	-5.0589439E-04	-1.4563385E-02	2.5061410E-01	
285	7.3499994E-01	-8.9341665E-06	6.0227820E-04	-1.0696676E-01	8.9685454E-02	
286	1.3694267E+00	9.7845165E-06	-7.2930002E-04	-3.4928272E-01	-9.3657675E-02	
287	2.5522453E+00	6.1678263E-06	1.2297876E-02	-4.9298781E-01	-1.6224526E-01	
288	4.7592004E+00	-9.5122511E-05	1.2306050E-01	-2.2981896E-01	-7.5638494E-02	
289	8.8821010E+00	-1.7044696E-03	4.0358527E-01	1.9020216E-01	4.6878442E-02	

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290	1.6598538E+01	-3.3490722E-02	4.5955502E-01	2.6898485E-01	7.0909914E-02
291	3.1079528E+01	-1.7976659E-01	1.4192470E-01	9.4582711E-02	2.5010988E-02
292	5.8358006E+01	-3.5445132E-01	-1.5547080E-01	-6.1021210E-02	-1.5051975E-02
293	1.1000966E+02	-3.3068223E-01	-1.8988192E-01	-8.3626235E-02	-2.1126171E-02
294	2.0848751E+02	-1.9048277E-01	-1.1074452E-01	-4.8575649E-02	-1.2239840E-02
295	3.9793692E+02	-8.1562455E-02	-4.7076496E-02	-2.0731398E-02	-5.2359922E-03
296	7.6660359E+02	-2.9130071E-02	-1.6474611E-02	-7.1776740E-03	-1.8063717E-03
297	1.4944323E+03	-9.6393649E-03	-5.4487794E-03	-2.3916031E-03	-6.0404305E-04
298	2.9570622E+03	-3.0667014E-03	-1.7080815E-03	-7.4001605E-04	-1.8594553E-04
299	5.9602824E+03	-1.0114887E-03	-5.6807403E-04	-2.4954728E-04	-6.3083197E-05
300	1.2287274E+04	-3.5232458E-04	-1.9484679E-04	-8.4131236E-05	-2.1116516E-05
301	2.6025475E+04	-1.2123834E-04	-6.7931142E-05	-2.9858569E-05	-7.5513692E-06
302	5.6920168E+04	-5.1206264E-05	-2.8281789E-05	-1.2218172E-05	-3.0678055E-06
303	1.2924147E+05	-1.2423186E-05	-6.9580184E-06	-3.0604736E-06	-7.7428947E-07
304	3.0640048E+05	-1.0166505E-05	-5.6313512E-06	-2.4435258E-06	-6.1470251E-07
305					
306					
307	3.2777475E-02	5.1272654E-08	-7.1337975E-08	-9.8695082E-08	1.5640040E-04
308	6.1052208E-02	9.4368734E-09	1.9756252E-07	4.1408779E-07	4.4494135E-04
309	1.1371780E-01	1.5149148E-07	-6.8163196E-07	-1.6165852E-06	9.9782587E-04
310	2.1181678E-01	1.7093311E-07	1.2680016E-06	-1.1699505E-06	1.4231482E-03
311	3.9455421E-01	5.8354045E-07	-3.3044203E-06	-8.8017777E-05	1.5196087E-03
312	7.3499994E-01	9.5286576E-07	4.2711904E-06	-8.8497625E-04	7.4213549E-04
313	1.3694267E+00	2.5613533E-06	-9.4734702E-06	-3.9447915E-03	-1.0579134E-03
314	2.5522453E+00	5.1356596E-06	1.8658384E-04	-7.6009953E-03	-2.5015174E-03
315	4.7592004E+00	9.4183882E-06	2.5869202E-03	-4.8349100E-03	-1.5912555E-03
316	8.8821010E+00	-2.4846844E-05	1.1600744E-02	5.4711831E-03	1.3487348E-03
317	1.6598538E+01	-1.2668094E-03	1.8043647E-02	1.0560150E-02	2.7838624E-03
318	3.1079528E+01	-9.5791864E-03	7.5931119E-03	5.0588871E-03	1.3376943E-03
319	5.8358006E+01	-2.5906001E-02	-1.1405232E-02	-4.4834319E-03	-1.1062167E-03
320	1.1000966E+02	-3.2939316E-02	-1.8940614E-02	-8.3445574E-03	-2.1081864E-03
321	2.0848751E+02	-2.5687730E-02	-1.4944831E-02	-6.5558307E-03	-1.6518885E-03
322	3.9793692E+02	-1.4730133E-02	-8.5051338E-03	-3.7462797E-03	-9.4625040E-04
323	7.6660359E+02	-6.8893687E-03	-3.8966271E-03	-1.6970918E-03	-4.2702250E-04
324	1.4944323E+03	-2.8874401E-03	-1.6343513E-03	-7.1820842E-04	-1.8148297E-04
325	2.9570622E+03	-1.0971088E-03	-6.1041945E-04	-2.6378718E-04	-6.6204885E-05
320	5.9602824E+03	-4.1131546E-04	-2.3233303E-04	-1.026/240E-04	-2.6017839E-05
220	1.2207274E+04	-1.4526502E-04	-7.9720102E-05	-3.4004690E-05	-0.4000/49E-00
320	5 6920168E+04	-3.3097340E-05	-9.8440828E-06	-1.3505000E-05	-3.4565051E-00
330	1 2924147E+05	-6 0357247E-06	-3 5020021E-06	-1 6064965E-06	-4 1341700E-07
331	3.0640048E+05	-2.7989375E-06	-1.5096828E-06	-6.3118668E-07	-1.5620812E-07
332					
333					
334		3D+	4D+	5D+	6D+
335		-1.2827939E+02	-2.6928655E+01	-3.8101969E+00	-1.8169381E-01
336					
337					
338	3.2777475E-02	-4.4802587E-07	2.4275314E-05	-7.5317133E-05	-1.0707794E-01
339	6.1052208E-02	1.6224646E-06	-8.3565772E-05	1.6617400E-04	-1.9937753E-01
340	1.1371780E-01	-3.3669023E-06	1.7587412E-04	-5.8806415E-04	-3.1991976E-01
341	2.11816/8E-01	5.6351388E-06	-2.9003014E-04	-7.3087509E-04	-3.15/05/2E-01
342	3.9455421E-01	-8.3286912E-06	4.6510025E-04	-1.86/6569E-02	-2.3125690E-01
343	1 369/267E+00	-1 521657/F-05	A 6523033E-04	-1.2503947E-01	1 0510492E-02
345	2 5522453E+00	-6 0920422F-06	-1 5488351F-02	-4 8552690F-01	1 5427095E-01
346	4.7592004E+00	1.3841937E-04	-1.4245950E-01	-1.8761814E-01	6.0618295E-02
347	8.8821010E+00	2.2622365E-03	-4.2633114E-01	2.1406810E-01	-5.2331763E-02
348	1.6598538E+01	4.0492708E-02	-4.4457077E-01	2.5889309E-01	-6.6387969E-02
349	3.1079528E+01	1.9887657E-01	-1.0644157E-01	7.5275550E-02	-1.9454885E-02
350	5.8358006E+01	3.6589928E-01	1.7260955E-01	-6.9603820E-02	1.6825684E-02
351	1.1000966E+02	3.2180831E-01	1.8693843E-01	-8.1980897E-02	2.0168569E-02
352	2.0848751E+02	1.7529852E-01	1.0234078E-01	-4.4647524E-02	1.0953251E-02
353	3.9793692E+02	7.0461699E-02	4.0733158E-02	-1.7825555E-02	4.3835269E-03
354	7.6660359E+02	2.2927985E-02	1.2979953E-02	-5.6181141E-03	1.3760728E-03
355	1.4944323E+03	6.6296509E-03	3.7587050E-03	-1.6416421E-03	4.0398079E-04
356	2.9570622E+03	1.7162680E-03	9.5520955E-04	-4.0992766E-04	1.0009302E-04
357	5.9602824E+03	4.3584798E-04	2.4710517E-04	-1.0871783E-04	2.6857714E-05
358	1.2287274E+04	1.0119312E-04	5.5350430E-05	-2.3344938E-05	5.6550027E-06
359	2.6025475E+04	2.4512440E-05	1.41209/3E-05	-0.3442033E-06	1.5822968E-06
300	5.6920168E+04	5.1949414E-06	2.1403391E-06	-1.1095423E-06	2.0310949E-07
260	1.2924147E+05	1.1521015E-00	0.099501/E-0/	-3.2300921E-07	0.2241922E-00
363		2 04000225-07	1 50000705-07	-6 0400260E-00	1 // 2 2 2 1 1 2 2 2 1 2 2 2 2 2 2 2 2 2
364	0100100102.00	3.0400933E-07	1.5808078E-07	-6.2498362E-08	1.4655020E-08
0.07	0100100102.00	3.0400933E-07	1.5808078E-07	-6.2498362E-08	1.4655020E-08
300	3.2777475E-02	3.0400933E-07 -2.5112890E-09	1.5808078E-07 4.1934348E-08	-6.2498362E-08	1.4655020E-08
366	3.2777475E-02 6.1052208E-02	3.0400933E-07 -2.5112890E-09 9.5532465E-09	1.5808078E-07 4.1934348E-08 -1.9775127E-07	-6.2498362E-08 -1.3098950E-07 3.9426617E-07	1.4655020E-08 -1.8714305E-04 -4.7556643E-04
365 366 367	3.2777475E-02 6.1052208E-02 1.1371780E-01	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03
365 366 367 368	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03
365 366 367 368 369	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -1.4022465E-03
365 366 367 368 369 370	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.3499994E-01	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06 -4.5883166E-06	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.0349402E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -1.4022465E-03 -5.2172390E-04
365 366 367 368 369 370 371	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349994E-01 1.3694267E+00	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06 -4.5883166E-06 5.2366233E-06	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.0349402E-03 -4.2269885E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414532E-03 -1.4026322E-03 -1.4022465E-03 -5.2172390E-04 1.1873505E-03
365 366 367 368 369 370 371 372	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.3499994E-01 1.3694267E+00 2.5522453E+00	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06 6.236233E-06 -2.3897014E-04	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.0349402E-03 -7.4874326E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -1.4022465E-03 -5.2172390E-04 1.1873505E-03 2.3788950E-03
305 366 367 368 369 370 371 372 373	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.7528844E-06	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 -4.5883166E-06 5.2366233E-06 -2.3897014E-04 -3.0018144E-03	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.0349402E-03 -4.2269885E-03 -7.4874326E-03 -3.9485289E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4022642E-03 -1.4022645E-03 -5.2172390E-04 1.1873505E-03 2.3788950E-03 1.2757083E-03
365 366 367 368 369 370 371 372 373 374	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.3499994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.752844E-06 6.5489371E-05	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06 4.588366E-06 5.2366233E-06 -2.3887014E-04 -3.001814E-03 -1.2268290E-02	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 3.2547256E-06 -1.324607E-04 -1.324607E-04 -1.324607E-03 -4.2269885E-03 -7.4874326E-03 -3.9465289E-03 6.1592757E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -5.2172390E-04 1.1873505E-03 2.3788950E-03 1.275708E-03 -1.5057738E-03
365 366 367 368 369 370 371 372 373 374 375	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.3499994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00 1.6598538E+01	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.7528844E-06 6.5489371E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.5963932E-03 4.2000E-05 1.596392E-05 4.2000E-05 1.596392E-05 4.2000E-05 1.596392E-05 4.2000E-05 1.596392E-	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06 5.2366233E-06 -2.3897014E-04 -3.0018144E-03 -1.2268290E-02 -1.7471504E-02 -0.277751204E-02 -1.7471504E-02	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.324607E-04 -1.32462885E-03 -7.4874326E-03 -3.9485289E-03 -6.15592757E-03 1.0170578E-02 -4.2000000000000000000000000000000000000	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -1.4022665E-03 -5.2172390E-04 1.1873505E-03 2.3788950E-03 1.2757083E-03 -1.5057738E-03 -2.6079155E-03 -2.6079155E-03
365 366 367 368 369 370 371 372 373 374 375 376	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349994E-01 1.3694267E+00 2.5522453E+00 4.759204E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01	3.0400933E-07 -2.5112890E-09 9.5532465E-09 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.7528844E-06 6.5489371E-05 1.5963932E-03 1.0724050E-02 0.0000000000000000000000000000000000	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 -2.388166E-06 5.2366233E-06 -2.3897014E-04 -3.0018144E-03 -1.2268290E-02 -1.7471504E-02 -5.6943677E-03	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.0349402E-03 -7.4874326E-03 -7.4874326E-03 -3.9485289E-03 6.1592757E-03 1.0170578E-02 4.0295907E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -1.402265E-03 -5.2172390E-04 1.1873505E-03 1.2757083E-03 1.5057738E-03 -1.5057738E-03 -1.6079155E-03 -1.0414543E-03 -1.0415543E-03 -1.0414543E-03 -1.0414543E-03 -1.0414543E-03 -1.0414543E-03 -1.0414543E-03 -1.05155E-03 -1.05155E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.05155E-03 -1.05155E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.041555555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.04155555E-03 -1.041555555E-03 -1.041555555E-03 -1.04155555555555555555555555555555555555
365 366 367 368 369 370 371 372 373 374 375 376 377 377	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349994E-01 1.3694267E+00 2.5522453E+00 4.759204E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01 5.835800EE+01	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.7528844E-06 6.5489371E-05 1.5963932E-03 1.0724050E-02 2.6975934E-02 2.69759754E-02 2.69759754E-02 2.69759754E-02 2.69759754E-02 2.69759754E-02 2.69759754E-02 2.69759754E-02 2.69759754E-02 2.69759754E-02 2.697555555555555555555555555555555555555	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06 -4.5883166E-06 5.2366233E-06 -2.3897014E-04 -3.0018144E-03 -1.7471504E-02 -5.6943677E-03 1.2723409E-02 4.80477E-02 -5.6943677E-03 1.2723409E-02 4.80477E-02 -5.6943677E-03 1.2723409E-02 -5.6943677E-03 1.2723409E-02 -5.6943677E-03 -5.69457E-03 -5.69457E-03 -	-6.2498362E-08 -1.3098950E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-03 -1.0349402E-03 -7.4874326E-03 -3.9485289E-03 6.1592757E-03 1.0170578E-02 4.0295907E-03 -5.1328540E-03 -5.1528540E-03 -	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4022426E-03 -5.2172390E-04 1.1873505E-03 2.3788950E-03 1.2757083E-03 -1.0614543E-03 1.26079155E-03 -1.0414543E-03 1.2409059E-03
365 366 367 368 369 370 371 372 373 374 375 376 377 378 370	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.3499994E-01 1.3694267E+00 2.5522453E+00 4.759204E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01 5.8358006E+01 1.100966E+02 2.0647E+E-02	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.752844E-06 6.5489371E-05 1.5963932E-03 1.0724050E-02 2.6975934E-02 3.2419769E-02 2.411972E-00	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 2.8124617E-06 5.2366233E-06 -2.3897014E-04 -3.001814E-03 -1.2268290E-02 -1.7471504E-02 5.6943677E-03 1.2723409E-02 1.8801788E-02 1.404641E-02	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.0324902E-03 -4.2269885E-03 -7.4874326E-03 3.9485269E-03 -0.170578E-02 1.0170578E-02 -5.1328540E-03 -8.2428979E-03 -6.124809E-03 -8.2428979E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -5.2172390E-04 1.1873505E-03 -5.2172390E-04 1.2757083E-03 -1.5057738E-03 -2.6079155E-03 -1.0414643E-03 1.2409059E-03 2.0278041E-03
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.3499994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 8.8821010E+00 1.6598538E+01 3.1079528E+01 1.1000966E+02 2.0848751E+02 2.0848751E+02 3.973607E+02	3.0400933E-07 -2.5112890E-09 9.5532465E-09 -2.2638410E-08 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.7528844E-06 6.5489371E-05 1.5963932E-03 1.0724050E-02 3.2419769E-02 2.4114276E-02 1.310704E-02	1.5808078E-07 4.1934348E-08 -1.9775127E-07 -1.2834203E-06 2.8124617E-06 6.2366233E-06 -2.3887014E-04 -3.0018144E-03 -1.2268290E-02 -1.7471504E-02 -5.6943677E-03 1.2723409E-02 1.8801788E-02 1.4046415E-02 7.60070eex-02	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 -1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.03249402E-03 -4.2269885E-03 -3.9485289E-03 -6.1592757E-03 1.0170578E-02 4.0295907E-03 -5.1328540E-03 -5.1328540E-03 -6.1248988E-03 -6.3329827E-03 -6.3329827E-03 -6.3329827E-03 -6.3329827E-03 -6.332982E-03 -6.324292E-03 -6.324292E-03 -6.332982E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.324292E-03 -6.3242982E-03 -6.324292E-03 -6.3242982E-03 -7.3242828E-03 -7.4242982E-03 -7	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4026322E-03 -1.4022465E-03 -5.217230E-04 1.2757083E-03 -1.5057738E-03 -1.0515E-03 -1.0414543E-03 -1.0414543E-03 -1.2409059E-03 2.0278041E-03 1.5024841E-03 .502841E-03 .502841E-03
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381	3.2777475E-02 6.1052208E-02 1.1371780E-01 2.1181678E-01 3.9455421E-01 7.349994E-01 1.3694267E+00 2.5522453E+00 4.7592004E+00 3.822101E+00 3.1079528E+01 5.8358006E+02 2.0848751E+02 3.9793692E+02 3.9793692E+02	3.0400933E-07 -2.5112890E-09 9.553245E-09 4.5049675E-08 -8.2213089E-08 1.4317164E-07 -2.4505475E-07 1.5406900E-08 2.7528844E-06 6.5489371E-05 1.5963932E-03 1.0724050E-02 2.6975934E-02 3.2419769E-02 2.4114276E-02 1.3197018E-02 5.8221774E-03	1.5808078E-07 4.1934348E-08 -1.9775127E-07 5.6940672E-07 -1.2834203E-06 -2.3897014E-04 -3.0018144E-03 -1.2268208E-02 -1.7471504E-02 -5.6943677E-03 1.2723409E-02 1.8801788E-02 1.801788E-02 1.4046415E-02 7.6097968E-03 3.286257E-03	-6.2498362E-08 -1.3098950E-07 3.9426617E-07 1.9101004E-06 -3.2547256E-06 -1.1324607E-04 -1.0349402E-03 -7.4874326E-03 -7.4874326E-03 -3.9485289E-03 -1.0170578E-02 4.0295907E-03 -5.1328540E-03 -8.2428979E-03 -6.1248998E-03 -3.3285423E-03 -1.4212514E-03	1.4655020E-08 -1.8714305E-04 -4.7556643E-04 -1.0414533E-03 -1.4022652E-03 -5.2172390E-04 1.187350EE-03 -1.5057738E-03 -1.5057738E-03 -1.0414543E-03 1.2409059E-03 -1.5024841E-03 8.1849208E-04

382	1.4944323E+03	2.2707250E-03	1.2839997E-03	-5.6067292E-04	1.3798793E-04
383	2.9570622E+03	7.8370384E-04	4.3440158E-04	-1.8606588E-04	4.5400882E-05
384	5.9602824E+03	2.6332078E-04	1.4918807E-04	-6.5774960E-05	1.6268067E-05
385	1.2287274E+04	7.8488463E-05	4.2535433E-05	-1.7781357E-05	4.2895664E-06
386	2 6025475E+04	2 4632134E-05	1 4332594E-05	-6.5269824E-06	1.6378398E-06
387	5 6020168E+04	6 0733526E-06	3 0796907E-06	-1 17/7621E-06	2 7012610E-07
200	1 0004147E+0E	1 9421000E-06	1 15720005-06	-E 7002080E-07	1 47702555-07
200	2 06400495+05	1.0401203E 00	0.0004107E-07	-6 4401020E-09	1 2066270E-09
209	3.0640046E+05	4.3591634E-07	2.00241276-07	-0.4421032E-08	1.32003/06-08
390					
391					
392		4F-	5F-		
393		-1.4283216E+01	-2.9142420E-01		
394					
395					
396	3.2777475E-02	-1.0725471E-05	1.8335167E-03		
397	6.1052208E-02	3.7371756E-05	1.4299458E-02		
398	1.1371780E-01	-6.5117205E-05	5.1474113E-02		
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401	7.3499994E-01	3.9034287E-04	2.8704100E-01		
402	1 3694267E+00	1 87110/25-03	3 1098500E-01		
402	2 EE224E2E+00	0.04950005-00	0.2016164E_01		
403	2.3322433E+00	2.9403902E-02	2.3910104E-01		
404	4.7592004E+00	1.3401088E-01	9.8299863E-02		
405	8.8821010E+00	2.9018994E-01	-3.8916120E-02		
406	1.6598538E+01	3.4836741E-01	-9.0866778E-02		
407	3.1079528E+01	2.6972459E-01	-7.6747815E-02		
408	5.8358006E+01	1.4163449E-01	-4.1716302E-02		
409	1.1000966E+02	5.3462215E-02	-1.5589750E-02		
410	2.0848751E+02	1.6463172E-02	-4.8330990E-03		
411	3.9793692E+02	4.0383670E-03	-1.1670891E-03		
412	7 6660359E+02	9 6404242E-04	-2 8455384E-04		
413	1 4944323F+03	2 0990334F-04	-5 9438911E-05		
414	0.05706005+02	4 0720190E-0E	-1 20E0110E-0E		
414	2.95/0622E+03	4.2/39109E-05	-1.2950119E-05		
410	5.9602824E+03	1.5565905E-05	-4.3943503E-06		
416					
417					
418	3.2777475E-02	-2.0783188E-08	3.6300411E-06		
419	6.1052208E-02	9.3085995E-08	3.8674853E-05		
420	1.1371780E-01	-2.3659580E-07	1.8998293E-04		
421	2.1181678E-01	6.3262257E-07	5.9574736E-04		
422	3.9455421E-01	-1.0880802E-06	1.4323838E-03		
423	7.3499994E-01	3.4104055E-06	2.6933700E-03		
424	1.3694267E+00	2.3452890E-05	3.9826033E-03		
425	2.5522453E+00	5.1386501E-04	4.1805895E-03		
426	4 7592004F+00	3 1956728E-03	2 3449523E-03		
497	9 9901010E+00	0.45151695-02	_1 0600000E_02		
421	1 6E00E20E+01	1 E402204E-00	-1.2000020E-03		
420	1.0390530E+01	1.0493324E-02	-4.0424051E-05		
429	3.10/9526E+01	1.030/503E-02	-4.0502595E-03		
430	5.8358006E+01	1.1/12012E-02	-3.4499746E-03		
431	1.1000966E+02	6.0012126E-03	-1.7499308E-03		
432	2.0848751E+02	2.4902691E-03	-7.3123932E-04		
433	3.9793692E+02	8.0917742E-04	-2.3369431E-04		
434	7.6660359E+02	2.5236369E-04	-7.4645254E-05		
435	1.4944323E+03	6.5321088E-05	-1.8336818E-05		
436	2.9570622E+03	1.7865583E-05	-5.4973542E-06		
437	5.9602824E+03	5.2672434E-06	-1.4302192E-06		
438					
439					
440		4F+	5F+		
441		-1.3898700E+01	-2.6933365E-01		
442					
443					
444	3 2777475F-02	1 1675980F-05	-2 6792931F-03		
445	6.1052208F-02	-4.1377000F-05	-1.7785577F-02		
446	1 13717805-01	7 08571048-05	-5 8567071E-02		
147	0 11012702-01	-1 /7086505-04	-1 0737200E_01		
441	2.11010/8E-01	1 6044060E 04	1.213130UE-U1		
440	3.3400421E-01	-1.0044202E-04	2.1040329E-01		
449	1.3499994E-01	-4.2099/UbE-04	-2.0/94124E-01		
400	1.309420/1400	-2.1/0/351E-03	-3.0039932E-01		
451	2.5522453E+00	-3.2039098E-02	-2.3140727E-01		
452	4.7592004E+00	-1.4005668E-01	-8.9645492E-02		
453	8.8821010E+00	-2.9608946E-01	4.2772328E-02		
454	1.6598538E+01	-3.4809129E-01	9.0168542E-02		
455	3.1079528E+01	-2.6411894E-01	7.4324210E-02		
456	5.8358006E+01	-1.3656877E-01	3.9659289E-02		
457	1.1000966E+02	-5.0325596E-02	1.4467214E-02		
458	2.0848751E+02	-1.4919582E-02	4.3176435E-03		
459	3.9793692E+02	-3.4681534E-03	9.8742386E-04		
460	7.6660359E+02	-7.6780228E-04	2.2383383E-04		
461	1.4944323E+03	-1.3866054E-04	3.8326704E-05		
462	2.9570622E+03	-2.6734026E-05	8.1305216E-06		
463	5.9602824E+03	-5.2648888E-06	1.3970692E-06		
464	5.0002024E-03	5.20-10000E 00	1.00100021 00		
465					
400	3 07774755 00	2 40201048 00	-5 30001638 00		
400	5.2///4/5E-02	2.4030104E-08	0.0099103E-06		
407	0.1052208E-02	-1.1408//1E-07	-4.81U2/4/E-05		
408	1.13/1/80E-01	2.0/15090E-07	-∠.1018653E-04		
469	2.1181678E-01	-1.5061919E-07	-6.4167480E-04		
470	3.9455421E-01	1.1736847E-06	-1.4814308E-03		
471	7.3499994E-01	-4.0316229E-06	-2.7020456E-03		
-					
472	1.3694267E+00	-2.7854269E-05	-3.9245322E-03		

474	4 7592004E+00 -3 3449889E-03 -2 1394404E-03
475	8.8821010E+00 -9.6582637E-03 1.3958154E-03
476	1.6598538E+01 -1.5510672E-02 4.0174278E-03
477	3.1079528E+01 -1.6082860E-02 4.5249404E-03
478	5.8358006E+01 -1.1361507E-02 3.2985776E-03 1 1000966E+02 -5 7154982E-03 1 6425083E-03
480	2.0848751E+02 -2.3118320E-03 6.6885753E-04
481	3.9793692E+02 -7.2978324E-04 2.0764163E-04
482	7.6660359E+02 -2.1946679E-04 6.4005928E-05
484	2.9570622E+03 -1.4013535E-05 4.2861177E-06
485	5.9602824E+03 -3.3747959E-06 8.7670867E-07
486	
487	Colouisted energy =
489	Literature energy = -2.72743775461054105410540
490	Difference (cal - lit) = 1.36E-03
491	Relative error (abs((cal - lit)/lit)) = 4.99E-08
492	35 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
494	3.2777474514072306E-02 1.0d0 1.0d0
495	6.1052208024089318E-02 1.0d0 1.0d0
490	2.1181678224305334E-01 1.0d0 1.0d0
498	3.9455421330447510E-01 1.0d0 1.0d0
499	7.3499993917294237E-01 1.0d0 1.0d0
500	1.3694267119018748E+00 1.0d0 1.0d0 2 5522453323068639E+00 1.0d0 1.0d0
502	4.7592004160127050E+00 1.0d0 1.0d0
503	8.8821010163462422E+00 1.0d0 1.0d0
504	1.6598538397889143E+01 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0
505	5.8358006063602978E+01 1.0d0 1.0d0
507	1.1000966104096939E+02 1.0d0 1.0d0
508	2.0848750508658674E+02 1.0d0 1.0d0
510	7.6660358942891128E+02 1.0d0 1.0d0
511	1.4944323346681333E+03 1.0d0 1.0d0
512	2.9570621576747585E+03 1.0d0 1.0d0
514	1.2287273922270530E+04 1.0d0 1.0d0
515	2.6025474503929181E+04 1.0d0 1.0d0
516	5.6920167949008617E+04 1.0d0 1.0d0
517	1.2924146561822579E+05 1.0d0 1.0d0 3.0640047899595002E+05 1.0d0 1.0d0
519	7.6297421342751326E+05 1.0d0 1.0d0
520	2.0076698631188064E+06 1.0d0 1.0d0
521	5.6164425941082174E+06 1.0d0 1.0d0 1.6802885560418982E+07 1.0d0 1.0d0
523	5.4065392869313173E+07 1.0d0 1.0d0
524	1.8809445122304142E+08 1.0d0 1.0d0
525	7.1100930633447683E+08 1.0d0 1.0d0 2.9330970963636436E+09 1.0d0 1.0d0
527	1.3255935848588299E+10 1.0d0 1.0d0
528	6.5852664686153687E+10 1.0d0 1.0d0
529	30 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
531	6.1052208024089318E-02 1.0d0 1.0d0
532	1.1371779544172864E-01 1.0d0 1.0d0
533	2.1181678224305334E-01 1.0d0 1.0d0 3.9455421330447510E-01 1.0d0 1.0d0
535	7.3499993917294237E-01 1.0d0 1.0d0
536	1.3694267119018748E+00 1.0d0 1.0d0
537	2.5522453323068639E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0
539	8.8821010163462422E+00 1.0d0 1.0d0
540	1.6598538397889143E+01 1.0d0 1.0d0
541 542	3.1079527707765703E+01 1.0d0 1.0d0 5.8358006063602978E+01 1.0d0 1.0d0
543	1.1000966104096939E+02 1.0d0 1.0d0
544	2.0848750508658674E+02 1.0d0 1.0d0
545	3.9793692474094433E+02 1.0d0 1.0d0
$540 \\ 547$	1.4944323346681333E+03 1.0d0 1.0d0
548	2.9570621576747585E+03 1.0d0 1.0d0
549	5.9602824302208819E+03 1.0d0 1.0d0
551	1.2207273922270530E+04 1.0d0 1.0d0 2.6025474503929181E+04 1.0d0 1.0d0
552	5.6920167949008617E+04 1.0d0 1.0d0
553	1.2924146561822579E+05 1.0d0 1.0d0
$554 \\ 555$	3.0640047899595002E+05 1.0d0 1.0d0 7.6297421342751326E+05 1 0d0 1 0d0
556	2.0076698631188064E+06 1.0d0 1.0d0
557	5.6164425941082174E+06 1.0d0 1.0d0
558 559	1.6802885560418982E+07 1.0d0 1.0d0 5 4065392869313173E+07 1.0d0 1.0d0
560	30 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
561	3.2777474514072306E-02 1.0d0 1.0d0
562 563	6.1052208024089318E-02 1.0d0 1.0d0 1 1371779544172864E-01 1.0d0 1.0d0
564	2.1181678224305334E-01 1.0d0 1.0d0
565	3.9455421330447510E-01 1.0d0 1.0d0

566		7.3499993917294237E-01 1.0d0 1.0d0							
567		1.3694267119018748E+00 1.0d0 1.0d0							
568		2.5522453323068639E+00 1.0d0 1.0d0							
570		8.8821010163462422E+00 1.0d0 1.0d0							
571		1.6598538397889143E+01 1.0d0 1.0d0							
572		3.1079527707765703E+01 1.0d0 1.0d0							
573		5.8358006063602978E+01 1.0d0 1.0d0							
574		1.1000966104096939E+02 1.0d0 1.0d0 2.0848750508658674E+02 1.0d0 1.0d0							
576		3.9793692474094433E+02 1.0d0 1.0d0							
577		7.6660358942891128E+02 1.0d0 1.0d0							
578		1.4944323346681333E+03 1.0d0 1.0d0							
579		2.9570621576747585E+03 1.0d0 1.0d0							
581		1 2287273922270530E+04 1 0d0 1 0d0							
582		2.6025474503929181E+04 1.0d0 1.0d0							
583		5.6920167949008617E+04 1.0d0 1.0d0							
584		1.2924146561822579E+05 1.0d0 1.0d0							
586		3.0640047899595002E+05 1.0d0 1.0d0 7.6297421342751326E+05 1.0d0 1.0d0							
587		2.0076698631188064E+06 1.0d0 1.0d0							
588		5.6164425941082174E+06 1.0d0 1.0d0							
589		1.6802885560418982E+07 1.0d0 1.0d0							
590	05	5.4065392869313173E+07 1.0d0 1.0d0			4				
591	25	3.2777474514072306E=02.1.0d0.1.0d0	1	1	T	1	1	1	T
593		6.1052208024089318E-02 1.0d0 1.0d0							
594		1.1371779544172864E-01 1.0d0 1.0d0							
595		2.1181678224305334E-01 1.0d0 1.0d0							
596		3.9455421330447510E-01 1.0d0 1.0d0 7.3409093017204237E-01 1.0d0 1.0d0							
598		1.3694267119018748E+00 1.0d0 1.0d0							
599		2.5522453323068639E+00 1.0d0 1.0d0							
600		4.7592004160127050E+00 1.0d0 1.0d0							
601		8.8821010163462422E+00 1.0d0 1.0d0							
602		1.6598538397889143E+01 1.0d0 1.0d0							
604		5.8358006063602978E+01 1.0d0 1.0d0							
605		1.1000966104096939E+02 1.0d0 1.0d0							
606		2.0848750508658674E+02 1.0d0 1.0d0							
607		3.9793692474094433E+02 1.0d0 1.0d0							
600		1 4944323346681333E+03 1 0d0 1 0d0							
610		2.9570621576747585E+03 1.0d0 1.0d0							
611		5.9602824302208819E+03 1.0d0 1.0d0							
612		1 2287273922270530F+04 1 0d0 1 0d0							
012		1.22012100222100001.04 1.040 1.040							
613		2.6025474503929181E+04 1.0d0 1.0d0							
613 614 615		2.6025474503929181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0							
613 614 615 616		2.6025474503929181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924145561822579E+05 1.0d0 1.0d0 3.0640047899595002E+05 1.0d0 1.0d0							
613 614 615 616 617	25	2.6025474503929181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 3.064004789555002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1	1	1	1	1	1	1
612 613 614 615 616 617 618	25	2.6025474503929181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 3.0640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620	25	2.6025474503929181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 3.0640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621	25	2.6025474503929181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 3.0640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622	25	2.6025474503829181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622 623	25	2.6025474503829181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 3.9455421304475105-01 1.0d0 1.0d0 7.3499993917294237E-01 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622 623 624 625	25	2.6025474503329181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 3.0640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.105220824089318E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 7.3499993917294237E-01 1.0d0 1.0d0 1.3642267119018748E+00 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622 623 624 625 626	25	2.6025474503329181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.105220620408318E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 3.9455421330447510E-01 1.0d0 1.0d0 1.3694267119018748E+00 1.0d0 1.0d0 2.5522453323068639E+00 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627	25	1.2007/05/2003/05/10/03/05/05/05/05/05/05/05/05/05/05/05/05/05/	1	1	1	1	1	1	1
612 613 614 615 616 617 618 620 621 622 623 624 625 626 627 628	25	1.2007/05/2003/05/10/03/05/05/05/05/05/05/05/05/05/05/05/05/05/	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630	25	2.6025474503329181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 3.9455421330447510E-01 1.0d0 1.0d0 1.3694267119018748E+00 1.0d0 1.0d0 1.369426719018748E+00 1.0d0 1.0d0 2.5522453323068639E+00 1.0d0 1.0d0 8.8821010163462422E+00 1.0d0 1.0d0 8.8821010163462422E+00 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631	25	2.6025474503829181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 3.9455421330447510E-01 1.0d0 1.0d0 1.3694267119018748E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 4.659853837889143E+01 1.0d0 1.0d0 3.86594297107765703E+01 1.0d0 1.0d0 5.8358006063602978E+01 1.0d0 1.0d0 5.8358006063602978E+01 1.0d0 1.0d0	1	1	1	1	1	1	1
612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632	25	2.6025474503829181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 3.0640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 1.0320204083318E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 7.3499993917294237E-01 1.0d0 1.0d0 7.3499993917294237E-01 1.0d0 1.0d0 7.3499993323068639E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 8.8821010163462422E+00 1.0d0 1.0d0 1.659853839789143E+01 1.0d0 1.0d0 3.0079E27707765703E+01 1.0d0 1.0d0 5.8388006063602978E+01 1.0d0 1.0d0 1.000966104096939E+02 1.0d0 1.0d0 1.000966104096932E+02 1.0d0 1.0d0	1	1	1	1	1	1	1
613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633	25	2.6025474503329181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 3.9455421304475105-01 1.0d0 1.0d0 2.5522453320648639E+00 1.0d0 1.0d0 2.5522453320648639E+00 1.0d0 1.0d0 2.552245332068639E+00 1.0d0 1.0d0 2.652245332068639E+00 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0 5.8358006063602978E+01 1.0d0 1.0d0 5.8358006063602978E+01 1.0d0 1.0d0 2.100966104096939E+02 1.0d0 1.0d0 3.0096508685674E+02 1.0d0 1.0d0 3.9793692474094433E+02 1.0d0 1.0d0	1	1	1	1	1	1	1
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613 613 614 615 616 617 618 620 621 622 623 624 625 626 625 626 627 628 629 630 631 632 633 634 635	25	2.6025474503329181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 3.9455421330447510E-01 1.0d0 1.0d0 1.3694267119018748E+00 1.0d0 1.0d0 1.369426719018748E+00 1.0d0 1.0d0 3.6592453323068639E+00 1.0d0 1.0d0 3.85204160127050E+00 1.0d0 1.0d0 8.882101013462422E+00 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0 3.1096104096939E+02 1.0d0 1.0d0 3.9793692474094433E+02 1.0d0 1.0d0 3.9793692474094432E+02 1.0d0 1.0d0 3.9793692474094432E+02 1.0d0 1.0d0 3.4039432346681332E+03 1.0d0 1.0d0	1	1	1	1	1	1	1
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613 613 614 615 616 617 618 619 620 621 622 622 622 622 622 622 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638	25	2.6025474503829181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 6.1052208024089318E-02 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 3.9455421330447510E-01 1.0d0 1.0d0 7.3499993917294237E-01 1.0d0 1.0d0 7.3499993917294237E-01 1.0d0 1.0d0 7.552243523068639E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 8.8821010163462422E+00 1.0d0 1.0d0 5.85326337889143E+01 1.0d0 1.0d0 5.8358006063602978E+01 1.0d0 1.0d0 5.8358006063602978E+01 1.0d0 1.0d0 5.835800663602978E+01 1.0d0 1.0d0 5.835802474094433E+02 1.0d0 1.0d0 3.0793692474094433E+02 1.0d0 1.0d0 1.4944323346681332E+03 1.0d0 1.0d0 1.4944322346681332E+03 1.0d0 1.0d0 5.9602824302208819E+03 1.0d0 1.0d0	1	1	1	1	1	1	1
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612 613 614 615 616 617 618 619 622 623 624 625 626 627 628 626 627 628 630 631 632 633 634 635 6364 637 638 639 634 635 638 639 634 635 638 639 634 635 638 639 634 635 636 637 638 639 634 635 638 639 634 635 638 639 638 639 638 639 638 639 638 639 638 639 638 639 638 639 638 639 638 639 634 638 639 634 638 639 634 638 639 638 639 640 641	25	1.2007/05/2003/05/07/05/03/07/07/05/03/07/05/05/07/05/05/07/05/05/07/05/05/07/05/05/05/05/05/05/05/05/05/05/05/05/05/	1	1	1	1	1	1	1
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613 613 614 615 616 616 617 618 620 621 622 623 624 625 626 625 626 627 628 629 630 631 632 633 633 634 635 636 637 638 639 640 641 642 639 640 641 642 632 633 634 635 636 637 638 639 640 641 641 642 632 632 633 634 635 636 637 638 639 640 641 642 643 644 645 636 637 638 636 637 638 636 637 638 639 640 641 642 643 644 645 645 645 645 645 645 636 637 638 638 639 640 641 642 643 645	25	12.2017.022474503329181E+04 1.0d0 1.0d0 5.6920167949008617E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.30640047399595002E+05 1.0d0 1.0d0 1.11 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 1.0371779544172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 1.3694527119018748E+00 1.0d0 1.0d0 1.3694267119018748E+00 1.0d0 1.0d0 1.5522453323068639E+00 1.0d0 1.0d0 2.5522453323068639E+00 1.0d0 1.0d0 2.652245323068639E+00 1.0d0 1.0d0 2.652245323068639E+00 1.0d0 1.0d0 2.652245323068639E+00 1.0d0 1.0d0 2.652245323068639E+00 1.0d0 1.0d0 3.8358006063602978E+01 1.0d0 1.0d0 1.000966104096939E+02 1.0d0 1.0d0 3.979369247409443E+02 1.0d0 1.0d0 3.979369247409443E+02 1.0d0 1.0d0 2.9570621576747585E+03 1.0d0 1.0d0 2.9570621576747585E+03 1.0d0 1.0d0 2.9570621576747585E+03 1.0d0 1.0d0 2.6025474503929181E+04 1.0d0 1.0d0 2.6026474503929181E+04 1.0d0 1.0d0 2.6026744503929602E75 1.0d0 1.0d0 2.602674503929602E75 1.0d0 1.0d0 2.602674504078755002E-05 1.0d0 1.0d0 2.602674504078755002E-05 1.0d0 1.0d0 2.602674504078755002E-05 1.0d0 1.0d0 2.602674504078755002E-05 1.0d0 1.0d0 2.602674504078755002E-05 1.0d0 1.0d0 2.602674504078755002E-05 1.0d0 1.0d0 2.60267450400478555002E-05	1	1	1	1	1	1	1
613 613 614 615 616 617 618 620 621 622 623 624 625 626 626 627 628 626 626 626 626 633 634 633 634 635 636 636 637 638 639 640 641 642 643 644 643	25	1.2007/02/2003/03/04/04/04/04/04/04/04/04/04/04/04/04/04/	1	1	1	1	1	1	1
613 613 614 615 616 617 618 620 620 621 622 623 624 625 626 626 626 627 628 629 633 632 633 635 636 637 638 639 634 635 636 637 638 640 641 644 645 644	25	1.2007/02/2008/178-04 1.0d0 1.0d0 1.292146561822579E+05 1.0d0 1.0d0 1.292146561822579E+05 1.0d0 1.0d0 1.30640047899595002E+05 1.0d0 1.0d0 1.11 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.0d0 1.0d0 1.037177954172864E-01 1.0d0 1.0d0 2.1181678224305334E-01 1.0d0 1.0d0 1.3694267119018748E+00 1.0d0 1.0d0 1.3694267139047850E-01 1.0d0 1.0d0 1.3694267139047850E+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 3.8552433230686392+00 1.0d0 1.0d0 4.7592004160127050E+00 1.0d0 1.0d0 3.85820663802978E+01 1.0d0 1.0d0 3.1079527707765703E+01 1.0d0 1.0d0 3.0793692474094433E+02 1.0d0 1.0d0 3.0793692474094433E+02 1.0d0 1.0d0 1.287450508658674E+02 1.0d0 1.0d0 1.297762157677585E+03 1.0d0 1.0d0 1.2287273922270530E+04 1.0d0 1.0d0 3.9793692474094433E+02 1.0d0 1.0d0 1.2287273922270530E+04 1.0d0 1.0d0 1.228747459432E+02 1.0d0 1.0d0 1.228747459432E+02 1.0d0 1.0d0 1.228747459432E+02 1.0d0 1.0d0 1.228747459432E+02 1.0d0 1.0d0 1.2287474594432E+02 1.0d0 1.0d0 1.22874745944322208534E+01 1.0d0 1.0d0 1.2277474514072306E+02 1.0d0 1.0d0 1.211117754417286E+01 1.0d0 1.0d0 1.1104	1	1	1	1	1	1	1
$\begin{array}{c} 613\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 629\\ 620\\ 622\\ 623\\ 622\\ 623\\ 624\\ 625\\ 626\\ 627\\ 628\\ 636\\ 637\\ 638\\ 639\\ 634\\ 635\\ 636\\ 638\\ 639\\ 640\\ 642\\ 648\\ 645\\ 646\\ 647\\ 648\\ \end{array}$	25	1.2007/02/03/03/03/03/03/03/03/03/03/03/03/03/03/	1	1	1	1	1	1	1
613 613 614 615 616 617 618 620 621 622 623 624 625 626 627 632 633 634 635 636 637 638 636 637 638 636 637 638 636 641 642 643 644 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 647 648 648 648 648 648 645 648 648 648 645 648 645 648 645 648 645 648 648 645 648 645 648 648 645 648 645 648	25	1.2007/02/03/03/03/03/03/03/03/03/03/03/03/03/03/	1	1	1	1	1	1	1
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613 613 614 615 616 617 618 622 622 622 622 622 622 625 626 627 628 629 633 634 635 634 635 636 637 638 639 640 641 642 643 644 645 644 645 644 645 646 647 648 649 644 645 646 647 648 649 645 646 645 646 647 648 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 646 645 645 646 645 655 655 1000 1000 1000 1000 1000 1000 1000 1000	25	1220717022474503329181E+04 1.030 1.030 5.6920167949008617E+04 1.030 1.030 1.2924146561822579E+05 1.030 1.040 1.2924146561822579E+05 1.030 1.040 1.32777474514072306E-02 1.030 1.040 1.1311779544172864E-01 1.030 1.040 2.1181678224305334E-01 1.030 1.040 2.1181678224305334E-01 1.030 1.040 1.3694527119018748E+00 1.040 1.040 2.552245323068639E+00 1.040 1.040 2.552245323068639E+00 1.040 1.040 2.552245323068639E+00 1.040 1.040 2.552245323068639E+00 1.040 1.040 2.658253397889143E+01 1.040 1.040 2.658253397889143E+01 1.040 1.040 2.658253397889143E+01 1.040 1.040 3.8821010163462422E+00 1.040 1.040 3.8358006063602978E+01 1.040 1.040 3.8358006063602978E+01 1.040 1.040 3.979369247409443E+02 1.040 1.040 3.979369247409443E+02 1.040 1.040 2.0848750508658674E+02 1.040 1.040 2.9870621576747588E+03 1.040 1.040 2.9570621576747588E+03 1.040 1.040 2.9570621576747588E+03 1.040 1.040 2.660035894229112E+02 1.040 1.040 2.6920457450392181E+04 1.040 1.040 2.927449940381+02 1.040 1.040 2.9274499408617E+04 1.040 1.040 2.92744561822579E+05 1.040 1.040 2.6920457450392181E+04 1.040 1.040 2.181678224305334E-01 1.040 1.040 2.1816782243323068639E+00 1.040 1.040 2.5522453323068639E+00 1.040 1.040 2.5522453323068639E+00 1.040 1.040 2.5522453323068639E+00 1.040 1.040	1	1	1	1	1	1	1
$\begin{array}{c} 613\\ 613\\ 613\\ 614\\ 615\\ 616\\ 617\\ 618\\ 620\\ 622\\ 6223\\ 6226\\ 6225\\ 6266\\ 627\\ 628\\ 628\\ 629\\ 631\\ 632\\ 633\\ 634\\ 635\\ 636\\ 637\\ 638\\ 639\\ 640\\ 641\\ 642\\ 648\\ 649\\ 644\\ 645\\ 646\\ 650\\ 651\\ 655\\ 8\end{array}$	25	1.2007/02/03/03/03/04/04/04/04/04/04/04/04/04/05/03/05/05/05/05/05/05/05/05/05/05/05/05/05/	1	1	1	1	1	1	1
613 613 614 615 616 617 618 620 622 622 622 622 622 622 622 622 622 622 622 622 623 624 625 626 627 628 629 630 631 633 634 635 636 637 638 639 641 642 644 645 644 645 644 645 644 645 652 655	25	1.2007/02/2785/2006/178-1040 1.040 1.040 2.6025474503829181E+04 1.040 1.040 1.2924146561822579E+05 1.040 1.040 1.2924146561822579E+05 1.040 1.040 1.30640047899595002E+05 1.040 1.040 1.11 1 1 1 1 1 1 1 1 1 1 1 1 1 3.2777474514072306E-02 1.040 1.040 1.371779544172864E-01 1.040 1.040 2.1181678224305334E-01 1.040 1.040 1.3694267119018748E+00 1.040 1.040 3.9455421330447510E-01 1.040 1.040 3.9455421330467510E+00 1.040 1.040 4.7592004160127050E+00 1.040 1.040 3.8524673323068639E+00 1.040 1.040 3.1079527707765703E+01 1.040 1.040 3.1079527707765703E+01 1.040 1.040 3.1079527707765703E+01 1.040 1.040 3.0793692474094433E+02 1.040 1.040 3.9793692474094433E+02 1.040 1.040 3.9793692474094433E+02 1.040 1.040 3.9793692474094433E+02 1.040 1.040 3.9793692474094433E+02 1.040 1.040 3.9602387450508658674E+02 1.040 1.040 3.9793692474094433E+02 1.040 1.040 3.9602367450508E+04 1.040 1.040 3.9602824302208819E+03 1.040 1.040 3.064004789959502E+05 1.040 1.040 3.02947465182279E+05 1.040 1.040 3.02947450382181E+04 1.040 1.040 3.02947450382181E+04 1.040 1.040 3.064004789959502E+05 1.040 1.040 3.277747451407230E=02 1.040 1.040 3.27774745147284E=01 1.040 1.040 3.27774745147284E=01 1.040 1.040 3.27774745147284E=01 1.040 1.040 3.28247119018748E=00 1.040 1.040 3.28247119018748E=00 1.040 1.040 3.8821010163462422270 1.040 1.040 3.8821010163462422270 1.040 1.040 3.8821010163462422270 0.1040 1.040 3.8821010163462422200 1.040 1.040 3.8821010163462422200 1.040 1.040 3.8821010163462422200 1.040 1.040 3.8821010163462422200 1.040 1.040 3.8821010163462422200 1.040 1.040 3.8821010163462422200 1.040 1.	1	1	1	1	1	1	1
613 613 614 615 616 617 618 620 622 622 622 622 622 623 624 625 626 627 628 632 633 634 635 636 637 638 639 641 642 643 644 645 644 645 646 647 648 649 645 646 647 648 649 645 646 645 646 647 648 645 646 645 645 646 645 645 646 645 645 646 645 645 646 645 645 645 645 646 645 655	25	1.2001/02/2006/178 2.6025474503329181E+04 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.2924146561822579E+05 1.0d0 1.0d0 1.11 1.11 1.11 1.11 3.0640047899595002E+05 1.0d0 1.0d0 1.11 1.11 1.11 1.11 3.2777474514072306E-02 1.0d0 1.0d0 1.1371779544172864E-01 1.0d0 1.0d0 2.181678224305334E-01 1.0d0 1.0d0 3.9455421330447510E-01 1.0d0 1.0d0 1.3694267119018748E+00 1.0d0 1.0d0 2.5522453320668395F00 1.0d0 1.0d0 3.9455421330447510540 1.0d0 1.0d0 1.659853837889143E1 1.0d0 1.0d0 1.659853837889143E1 1.0d0 1.0d0 1.659853837889143E1 1.0d0 1.0d0 1.000966104096939E+02 1.0d0 1.0d0 1.000966104096939E+02 1.0d0 1.0d0 1.97976215767758E503 1.0d0 1.0d0 <t< th=""><th>1</th><th>1</th><th>1</th><th>1</th><th>1</th><th>1</th><th>1</th></t<>	1	1	1	1	1	1	1
613 613 614 615 616 617 618 620 622 623 624 622 623 624 625 626 627 632 633 634 635 636 637 644 645 644 645 644 645 644 645 644 645 644 645 657 657	25	1.2007/02/03/03/03/04/04/04/04/04/04/04/04/05/03/05/05/05/05/05/05/05/05/05/05/05/05/05/	1	1	1	1	1	1	1

658		2.0848750508658674E+02	1.0d0	1.0d0
659		3.9793692474094433E+02	1.0d0	1.0d0
660		7.6660358942891128E+02	1.0d0	1.0d0
661		1.4944323346681333E+03	1.0d0	1.0d0
662		2.9570621576747585E+03	1.0d0	1.0d0
663		5.9602824302208819E+03	1.0d0	1.0d0
664	20	1 1 1 1 1 1 1 1 1 1 1 1	111	11111
665		3.2777474514072306E-02	1.0d0	1.0d0
666		6.1052208024089318E-02	1.0d0	1.0d0
667		1.1371779544172864E-01	1.0d0	1.0d0
668		2.1181678224305334E-01	1.0d0	1.0d0
669		3.9455421330447510E-01	1.0d0	1.0d0
670		7.3499993917294237E-01	1.0d0	1.0d0
671		1.3694267119018748E+00	1.0d0	1.0d0
672		2.5522453323068639E+00	1.0d0	1.0d0
673		4.7592004160127050E+00	1.0d0	1.0d0
674		8.8821010163462422E+00	1.0d0	1.0d0
675		1.6598538397889143E+01	1.0d0	1.0d0
676		3.1079527707765703E+01	1.0d0	1.0d0
677		5.8358006063602978E+01	1.0d0	1.0d0
678		1.1000966104096939E+02	1.0d0	1.0d0
679		2.0848750508658674E+02	1.0d0	1.0d0
680		3.9793692474094433E+02	1.0d0	1.0d0
681		7.6660358942891128E+02	1.0d0	1.0d0
682		1.4944323346681333E+03	1.0d0	1.0d0
683		2.9570621576747585E+03	1.0d0	1.0d0
684		5.9602824302208819E+03	1.0d0	1.0d0

Listing A.6: Output file for calculating the single point energy of Pa using a predefined basis set.

Appendix B Scripts for cudaDFRATOM

These are the scripts for automating the optimization of basis sets using cudaDFRATOM.

#!/bin/bash sym='' nuc='' exepath=/home/dhenness/prophet/exe # path to the executable ver=dfratomgpu_binarysearch2.x # the cudaDFRATOM executable file alljobs=false bottom=false wtime=01:00:00 if [[-z \$exepath]]; then echo "You must set the path to the executable" exit fi while [\$# -gt 0] do val=\$1 shift case \$val in "-a") alljobs=true ;; "-b") bottom=true ;; "-gauss") nuc='gauss_' :: "-point") nuc='point_' ;; "-S") sym='S' low=\$1 high=\$2 shift shift ;; "**-**P") sym='P' low=\$1 high=\$2 shift shift ;; "-D") sym='D' low=\$1 high=\$2 shift shift ;; "-F") sym='F' low=\$1 high=\$2 shift shift ;; "-t") 61 62 63 wtime=\$1 shift

```
64
             ;;
*)
 65
66
              job=$val
 67
68
            ;;
       esac
 69
70
71
72
73
74
75
76
77
78
79
80
      done
      boilerplate(){
      cat << EOF
#!/bin/bash
      #SBATCH --account=def-mariusz
#SBATCH --gres=gpu:1
      #SBATCH --mem=4GB
#SBATCH --time=$1
      #SBATCH --job-name=$2
#SBATCH --output=%x-%j.out
 81
82
83
      echo -----
      echo -----
      echo began running on \'date\'
echo -----
 84
85
 86
      $3 $4 > $5
      echo -----
 87
88
      echo stopped running on \'date\'
echo -----
 89
90
91
92
93
94
95
      EOF
      }
      if [[ -z snuc ]]; then
 96
97
98
99
       echo No nuc entered
exit
      fi
100
      if [ "$alljobs" = true ]; then
      ii ( $$ airjobs - true ],
job='ls *inp'
elif [ -z "$job" ]; then
echo no job given
exit
fi
101
104 \\ 105
106
107
108
      for file in $job; do
    dir='echo $file | sed 's/_.*$//''
109
        mkdir $dir
       cp $file $dir/$file-orig
cd $dir
1112
112
113
114
115
116
       # keep old out files and delete others
rename "out" "out-old" *.out
        rm *inp
        rm *sh
117
118
119
        file_base=$(echo $file | sed -e "s/$nuc.*/$nuc/")
read -r -a old_bs <<< $(sed -n -e "/nbs/{s/nbs=//; p}" $file-orig)
read -r -a old_start <<< $(sed -n -e "/start/{s/start=//; s/\$end//; p}" $file-orig)</pre>
120
121
122
123
        # keep track of how many files are made
total=0
124 \\ 125
        for i in $(seq $low $high); do
           for j in $(seq 0 6); do
126
127
            new_bs[j]=${old_bs[j]}
              new_start[j]=${old_start[j]}
128
           done
129
130
           # make alterations based on symmetry
           case $sym in
132
133
              "F")
134
                 ((new_bs[5]-=$i))
                ((new_bs[6]-=$i))
                136
137
                  break
                fi
                ((new_start[5]+=$i))
((new_start[6]+=$i))
140
141
142
              ;;
"D")
143
144
                 ((new bs[3]-=$i))
                 ((new_bs[4]-=$i))
145
146 \\ 147
                if [[ "${new_bs[3]}" == "0" ]]; then
                  break
                fi
148
                ((new_start[3]+=$i))
((new_start[4]+=$i))
149
150
151
              ;;
"P")
                ((new_bs[1]-=$i))
154 \\ 155
                ((new_bs[2]-=$i))
if [[ "${new_bs[1]}" == "0" ]]; then
```

156	break
157	fi
158	((new_start[1]+=\$i))
159	((new_start[2]+=\$i))
160	
161	"S")
162	((new_bs[0]-=\$i))
163	if [["\${new_bs[0]}" == "0"]]; then
164	break
165	fi
166	((new_start[0]+=\$i))
167	;;
168	esac
169	new_file=\$file_base\${new_bs[0]}"s"\${new_bs[1]}"p-"\${new_bs[2]}"p+"\${new_bs[3]}"d-"\${new_bs[4]}"d+"\${new_bs[5]}"f-"\${new_bs[6]}"f+.inp"
170	cp \$file-orig \$new_file
171	sed -i -e "s/\${old_bs[0]} \${old_bs[1]} \${old_bs[2]} \${old_bs[3]} \${old_bs[4]} \${old_bs[5]} \${old_bs[6]}/\
172	<pre>\${new_bs[0]} \${new_bs[1]} \${new_bs[2]} \${new_bs[3]} \${new_bs[4]} \${new_bs[5]} \${new_bs[6]}/" \$new_file # continuing from last line</pre>
173	if ["\$bottom" == true]; then
174	sed -i -e "s/\${old_start[0]} \${old_start[1]} \${old_start[2]} \${old_start[3]} \${old_start[4]} \${old_start[5]} \${old_start[6]}/
175	<pre>\${new_start[0]} \${new_start[1]} \${new_start[2]} \${new_start[3]} \${new_start[4]} \${new_start[5]} \${new_start[6]}/" \$new_file # continuing from last</pre>
	line
176	fi
177	
178	bollerplate \$wtime \${new_file%????} \$exepath/\$ver \$new_file \${new_file%???}log > \${new_file%???}sh
100	((total++))
101	done
101	
102	anda "Chimitting Otatal innut filag"
184	echo submitting ecotal input illes
185	
186	
187	
±01	4440

Listing B.1: BS_sub_auto.sh: Generate and submit input files.

1
#!/bin/bash
2
tol=\$1
tol=\$1
if [-z \$tol]; then
tol='5*10^-8'
fi
echo The tolerance in relative error is \$tol
mkdir best
for dir in 'ls -d */'; do
if ["\$dir" != 'otol/']; then
if ["\$dir" != 'best/']; then
if ["\$dir" != 'best/']; then
cd \$dir
for file in *.inp; do
error='grep -i 'rela' \${file%????}*log | tail -1 | awk '{print \$7}''
compercor='cecho \$error | sed -e 's/E/(*10\^')'
testthress='echo "scale=20; (\$tol - \$compercor)*10^10 >= 1" | bc -1'
if [\$teetthress -ge 1]; then
cp \$file .../best
cp \${file}.../best
fi
done
fi
fi
fi
cd...
done

Listing B.2: BS_get_best.sh: Find the best basis set.