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THE UNIVERSITY OF ALBERTA

THE CHEMISTRY OF BINUCLEAR RHODIUM COMPLEXES  
WITH SMALL MOLECULES

by

©

STEPHEN KENNETH DWIGHT

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH  
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THE UNIVERSITY OF ALBERTA  
FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled The Chemistry of Binuclear Rhodium Complexes with Small Molecules submitted by Stephen Kenneth Dwight in partial fulfilment of the requirements for the degree of Doctor of Philosophy.

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To my wife, Maureen.

## ABSTRACT

An X-ray structural determination of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$  ( $\text{DPM} = \text{Ph}_2\text{PCH}_2\text{PPh}_2$ ), has indicated that in this "A-frame" complex both the enclosed bridging site and exposed terminal sites are open to attack by small molecules. Whereas, in *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$ , a structural determination has shown that the bridging site is effectively blocked by the equatorial ligands, in particular the chloro ligands are skewed into this site, leaving only the possibility of terminal attack.

Halide exchange reactions were carried out on *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  in an effort to prepare the bromo and iodo derivatives. Instead the complexes  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ , which was structurally characterized, and  $[\text{Rh}_2\text{I}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{I}]$  were isolated as the final products. Iodide exchange on *trans*- $[\text{RhCl}(\text{CO})(\text{DAM})]_2$  ( $\text{DAM} = \text{Ph}_2\text{AsCH}_2\text{-AsPh}_2$ ) yields a mixture of *trans*- $[\text{RhI}(\text{CO})(\text{DAM})]_2$  and  $[\text{Rh}_2\text{I}(\text{CO})(\mu\text{-CO})(\text{DAM})_2][\text{I}]$ .

The chemistry of these binuclear rhodium species with  $\text{CO}$ ,  $\text{CS}_2$  and  $\text{SO}_2$  was investigated. The "A-frame" species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$  undergoes a facile and reversible reaction with  $\text{SO}_2$  yielding  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\mu\text{-SO}_2)(\text{DPM})_2][\text{BPh}_4]$ . Spectroscopic studies indicate that attack by  $\text{SO}_2$  occurs directly at the bridging site. Treatment of this  $\text{SO}_2$  adduct with excess  $\text{SO}_2$  in the presence of chloride

ion or  $[\text{Rh}_2\text{Cl}_2(\text{CO})_2]^-$ , which functions as a chloride transfer agent, results in the isolation of a second product  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  whose structure has been determined. Reaction of either *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  or  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  with  $\text{SO}_2$  results finally in the isolation of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  and reaction schemes are presented for both these reactions based on spectroscopic evidence.

Treatment of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  with CO yields the tricarbonyl species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{Cl}]$ . Similarly the reaction of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  with excess CO also yields this tricarbonyl species. However on slow stepwise addition of CO, *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  is isolated. Reaction of a mixture of *trans*- $[\text{RhI}(\text{CO})(\text{DAM})]_2$  and  $[\text{Rh}_2\text{I}(\text{CO})(\mu\text{-CO})(\text{DAM})_2][\text{I}]$  with CO or  $\text{SO}_2$  yield the products  $[\text{Rh}_2(\text{CO})_2(\mu\text{-L})(\mu\text{-I})(\text{DAM})_2][\text{I}]$  ( $\text{L} = \text{CO}, \text{SO}_2$ ).

Although  $\text{CS}_2$  does not react with  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$ , its reaction with either *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  or  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  yields as the final product  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$ . A structural determination of this species has shown that two molecules of  $\text{CS}_2$  have condensed yielding a  $\text{C}_2\text{S}_4$  fragment which bridges the two rhodium centres such that a five membered  $\text{Rh-C-S-C-S}$  metallacycle and a four membered  $\text{Rh-C-S-Rh}$  metallocycle results. Reaction schemes for these reactions are presented based on spectroscopic data and analogies to  $\text{SO}_2$  and acetylene chemistry.

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## LIST OF ABBREVIATIONS

- Me = methyl  
Et = ethyl  
n-Pr = n-propyl  
i-Pr = iso-propyl  
n-Bu = n-butyl  
t-Bu = tert-butyl  
COD = 1,5 cyclooctadiene  
THF = tetrahydrofuran  
HFB = hexafluoro-2-butyne  
DMA = dimethylacetylenedicarboxylate  
DPM = bis(diphenylphosphino)methane  
DAM = bis(diphenylarsino)methane

## CHAPTER I.

### INTRODUCTION

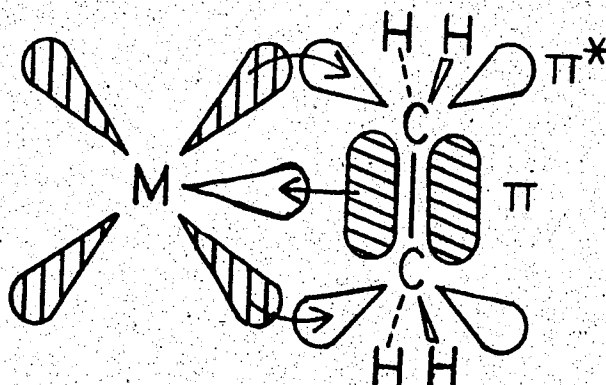
Homogeneous catalysis by transition metal complexes is currently, and has been for two decades, an area of considerable interest.<sup>1-4</sup> Several important successes have been achieved in this area translating homogeneously catalyzed reactions into viable commercial processes. Included among these are the Wacker process for olefin oxidation based on a palladium catalyst,<sup>5,6</sup> the hydroformylation process using a rhodium (I) phosphine complex<sup>7</sup> and the carbonylation of methanol to acetic acid employing a rhodium carbonyl iodide species.<sup>8,9</sup>

Many approaches have been used in catalytic studies, however it remains of fundamental importance to obtain an understanding of the chemical processes which occur at the metal centre during the catalytic reaction. Such information is required if one hopes intelligently to modify the catalyst's properties to achieve the results desired. With this objective in mind it becomes convenient to break the catalytic reaction down into three steps:<sup>10</sup> 1) substrate coordination and activation; 2) substrate transformation into product or product precursor; and 3) product elimination. If catalyst regeneration has not occurred a fourth step, that of catalyst regeneration, must also be added.

In catalytic reactions direct information about any of the above steps is, by the very nature of the catalytic process, limited. However, one approach which has proven useful, involves model system studies utilizing complexes which are similar to a given catalyst but which are not themselves catalysts.<sup>10-12</sup> By this approach useful analogies can be made between the model system and the related catalyst. It is obvious, therefore, that small molecule coordination in transition metal complexes and the activation of the small molecule by the metal centre are of interest in that these topics pertain to the first step in the above breakdown of catalytic reactions. It is on this theme, i.e. the coordination and activation of small molecules in transition metal complexes, that this thesis will concentrate.

In studies of small molecule coordination and activation, the initial step involves the coordination of the small molecule to a coordinately unsaturated metal centre. Here it is important to have a knowledge of how the small molecule coordinates in order to understand the resulting chemistry. Concurrent with coordination is activation of the small molecule, making it more reactive than it was prior to coordination. Activation results from a net change in the electron density distribution within the coordinated molecule. In molecular orbital terms this corresponds to electron donation from the substrate bonding

orbitals to the metal centre followed by back donation from the metal centre into orbitals which are antibonding in terms of the substrate bonds. The well known Dewar, Chatt, Duncanson<sup>13,14</sup> model for ethylene coordination to metals, which is diagrammed below, is a familiar example of this.



The bonding here is considered to consist of two interdependent components: 1) donation of  $\pi$ -electron density from the olefin to a  $\sigma$ -type acceptor orbital on the metal atom; and 2) back donation of electron density from filled metal  $dxz$  or other  $d\pi-p\pi$  hybrid orbitals into antibonding  $\pi^*$  orbitals of the olefin. Both components are synergically related, that is an increase in one component tends to promote an increase in the other and further both tend to decrease the bond order of the olefinic linkage. The structural results of this ethylene activation are well documented,<sup>15,16</sup> showing a lengthening of the C-C bond and a bending back of the hydrogen atoms away from the metal



centre. Clearly, a thorough understanding of this first important step in catalytic processes, that of substrate coordination and activation, is extremely important for a better understanding of these reactions.

In this thesis the small molecules whose transition metal chemistry will be pursued are carbon monoxide, carbon disulfide and sulfur dioxide. Each of these molecules has important relevance to catalysis. The catalyzed activation of carbon monoxide, for example, is of importance since the conversion of coal<sup>17</sup> to substitute natural gas, hydrocarbons and organic chemicals is based on the metal catalyzed reduction of carbon monoxide via methanation reactions and the Fischer-Tropsch synthesis.<sup>18-21</sup> Carbon disulfide activation, on the other hand, may serve as a useful model for the activation of the less reactive carbon dioxide molecule, which is an abundant potential feedstock for hydrocarbon production.<sup>10</sup> And with the increased utilization of coal, the deleterious effects of sulfur dioxide on the environment encourage efforts aimed at its removal. The use of transition metal catalysts for SO<sub>2</sub> removal from flue gases has proven useful in this regard.<sup>22-26</sup>

Furthermore, the three small molecules of interest are particularly germane to studies of small molecule coordination and activation since they each display a rich variety of coordination modes in metal complexes. Their study promises to yield valuable information relating these coordination modes to properties of the metal complexes, and

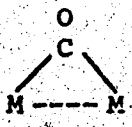
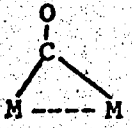
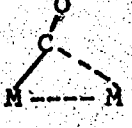
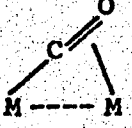
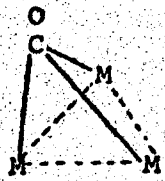
therefore promises to increase our understanding of factors affecting small molecule coordination and activation.

Insertion reactions of these small molecules other than into metal-metal bonds, although potentially important models for catalytic processes such as the Fischer-Tropsch synthesis,<sup>20,21</sup> the catalytic carbonylation of methanol to acetic acid,<sup>8</sup> and hydroformylation reactions,<sup>27,28</sup> will not be discussed here.

The carbonyl group, which has been extensively studied,<sup>10,29</sup> is found to be a tremendously versatile ligand displaying a wide variety of coordination modes. These modes, together with examples of each are presented in Figure 1. The first and most common bonding mode is that of the terminal carbonyl ligand. In this geometry the carbonyl group is associated with only one metal centre, is bound through the carbon atom and has an essentially linear M-C-O linkage.

The second class is that of the doubly bridging carbonyl group in which the carbonyl ligand is associated simultaneously with two metal centres. In this case classification is somewhat more complex than in the terminal class, since now the carbonyl ligand can display a significant range in coordination geometries. For the sake of convenience however, these ligands can be grouped into three classes; symmetrical, asymmetrical and semibridging. One method of distinguishing these three, somewhat arbitrary classes is based on metal-carbonyl bond distances. For the

Figure 1. Coordination Modes of the Carbonyl Ligand

Mode		Example	Reference
terminal	M-C-O	<i>trans</i> -[IrCl(CO) <sub>2</sub> (PPh <sub>3</sub> ) <sub>2</sub> ] <i>trans</i> -[RhCl(CO)(DAM)] <sub>2</sub>	30 31
symmetrical-μ <sub>2</sub>		[Pd <sub>2</sub> Cl <sub>2</sub> (μ-CO)(DAM) <sub>2</sub> ] [Fe <sub>2</sub> (CO) <sub>6</sub> (μ-CO)(DPM)]	32 33
asymmetrical-μ <sub>2</sub>		[Rh(CO)(μ-CO)(PPh <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> [Rh <sub>2</sub> (CO) <sub>2</sub> (μ-CO)(μ-Cl)(DPM) <sub>2</sub> ] <sup>+</sup>	34 35
semibridging-μ <sub>2</sub>		[Fe <sub>2</sub> (CO) <sub>5</sub> (μ-CO)(PhCCPh)]	36
linear-μ <sub>2</sub>		[Mn <sub>2</sub> (CO) <sub>4</sub> (μ-CO)(DPM) <sub>2</sub> ] <sup>-</sup>	37
triply-bridging		[Co <sub>6</sub> (CO) <sub>14</sub> ] <sup>4-</sup>	38

symmetrical species the metal-carbonyl distances differ by less than  $3\sigma$  where,  $\sigma = \sqrt{\sigma_a^2 + \sigma_b^2}$  and  $\sigma_a$  and  $\sigma_b$  are the standard deviations in the two metal-carbonyl bond lengths. The species within the semibridging group, on the other hand, are arbitrarily defined as having metal-carbonyl distances, which differ by greater than  $0.3 \text{ \AA}$ , and the third class, containing the asymmetrical species, between the two above extremes. In addition, a further distinction between these differing doubly bridging carbonyl geometries can be made based on the carbonyl C-O vector. In the symmetrical bridging mode the C-O vector is perpendicular to the M-M axis whereas in the asymmetrical and semibridging groups the C-O vector tends away from normality. Therefore, the closer the carbonyl geometry approaches the semibridging limit, the closer the M-C-O linkage is to being colinear with respect to the more strongly bound metal.

Another bridging carbonyl geometry, that of the linear- $\mu_2$ -bridging carbonyl mode, might be considered as a further extreme of the semibridging mode. In this carbonyl bonding mode the carbonyl ligand is  $\sigma$ -bound to one metal centre, resulting in an approximately linear M-C-O linkage and is simultaneously  $\pi$ -bound to a second metal centre. Unlike all previous carbonyl bonding modes, however, which function as two electron donors, this linear- $\mu_2$ -bridging ligand acts as a four electron donor.

The carbonyl ligand can also function as a triply bridging ligand having the carbonyl group simultaneously

associated with three metal centres. As with the doubly bridging carbonyl ligands, the triply bridging carbonyl group can be either symmetrical or asymmetrical.

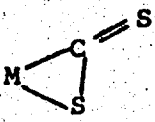
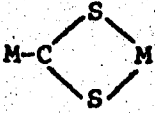
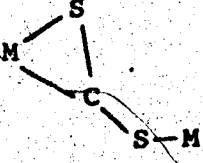
Until recently it was a well established dogma of transition metal carbonyl chemistry that bridging carbonyl groups were always accompanied by a metal-metal bond.<sup>39,40</sup> However, the recent structural characterizations of  $[\text{Pd}_2\text{Cl}_2(\mu\text{-CO})(\text{DAM})_2]$ ,<sup>32</sup>  $[\text{Pt}_2\text{Cl}_2(\mu\text{-CO})(\text{DAM})_2]$ <sup>41</sup> and  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\mu\text{-DMA})(\text{DPM})_2]$ <sup>42</sup> have shown that this is not the case. In each of the three complexes the metal-metal separation (ranging from 3.162(4)Å to 3.354(1)Å) is too long for a direct metal-metal interaction and the metal-carbonyl-metal angles are *ca.* 120°, contrasting with conventional bridging carbonyl ligands where angles between 62° and 90° are common.<sup>29</sup> The drawings in Figure 1, therefore, show dotted lines between the metal atoms to avoid implications regarding the presence or absence of a metal-metal bond.

The differentiation between the above carbonyl bonding modes can in general be conveniently carried out using infrared spectroscopy, since the carbonyl stretching frequencies for terminal carbonyl ligands are usually higher than those of doubly bridging carbonyl groups which are in turn higher than those for the triply bridging mode. However, differentiation between the types of doubly bridging modes presents a problem, since no obvious trend in their carbonyl stretching frequencies is observed. Thus, in

$[\text{Pt}_2\text{Cl}_2(\mu\text{-CO})(\text{DAM})_2]$ ,<sup>41</sup> which contains a symmetrical carbonyl ligand, the carbonyl frequency ( $1638\text{ cm}^{-1}$ ) is significantly different than that observed in the analogous palladium complex,  $[\text{Pd}_2\text{Cl}_2(\mu\text{-CO})(\text{DAM})_2]$  ( $1704\text{ cm}^{-1}$ ) but compares well with that of  $[\text{Mn}_2(\text{CO})_4(\mu\text{-CO})(\text{DPM})_2]$  ( $1645\text{ cm}^{-1}$ ),<sup>37</sup> which contains a linear- $\mu_2$ -bridging carbonyl group. It is relevant to discussions of carbonyl activation that the carbonyl stretching frequencies indicate an increase in activation (i.e. a decrease in C-O bond order) as the number of metal atoms associated with the ligand increases.

The carbon disulfide molecule also displays a variety of coordination modes, both in mononuclear and polynuclear species. Yet this small molecule has received relatively little attention with only a few species having been structurally characterized.<sup>43,44</sup> The three modes of carbon disulfide coordination which were structurally characterized at the time this research was undertaken are summarized in Figure 2. In the  $\text{C},\text{S}-\eta^2$  coordination geometry the carbon disulfide molecule is associated with only one metal centre, coordinating in a side-on manner via one of the sulfur atoms and the carbon atom. This is perhaps the commonest mode of  $\text{CS}_2$  coordination. In addition, two bridging geometries have been observed for the carbon disulfide ligand, shown in Figure 2 as modes A and B. Mode A has the carbon atom bound to one metal centre and the two sulfur atoms coordinated to the second metal centre;

Figure 2. Structurally Characterized Coordination Modes of Carbon Disulfide

	Mode	Example	Reference
C,S- $\eta^2$		$[\text{Pt}(\text{PPh}_3)_2(\text{CS}_2)]$	45
bridging A		$[\text{Pt}_2\text{Cl}(\text{CS}_2)(\text{PPh}_3)_4]^+$	46
bridging B		$(\text{PhMe}_2\text{P})_2(\text{CO})_2\text{Fe}(\text{CS}_2)\text{Mn}(\text{CO})_2\text{Cp}$	47



whereas mode B, has the  $\text{CS}_2$  ligand coordinated in an  $\text{C,S-}\eta^2$  fashion to one metal centre and via the second sulfur atom to the other metal centre.

Two other  $\text{CS}_2$  bonding modes have been proposed although these have not been structurally characterized. Coordination of  $\text{CS}_2$  through the sulfur atom ( $\text{M-S=C=S}$ ) has been suggested,<sup>48</sup> however these species tend to be poorly characterized. Condensation of the carbon disulfide molecules yielding a  $\text{C}_2\text{S}_5$  fragment has also been proposed in  $[\text{RhCl}(\text{PPh}_3)_2(\text{C}_2\text{S}_5)]$ <sup>49</sup> but characterization is again incomplete. In addition to these proposed coordination modes two others are possible based on analogies with  $\text{CO}_2$  chemistry. These involve either a  $\text{C}_2\text{S}_4$  fragment, resulting from the condensation of two  $\text{CS}_2$  molecules, analogous to the  $\text{C}_2\text{O}_4$  fragment observed in  $[\text{IrCl}(\text{C}_2\text{O}_4)(\text{PPh}_3)_2]$ ,<sup>50</sup> or an  $\eta^1$  carbon-bound species analogous to that proposed for  $\text{CO}_2$  coordination in  $[\text{Ni}(\text{CO}_2)(\text{P}(\text{n-Bu})_3)_3]$ .<sup>51</sup>

Correlations between the coordination mode of carbon disulfide and the infrared stretching frequencies have not been reported to date due to the limited structural data available. But again a significant drop in  $\text{CS}_2$  stretching frequencies is observed on coordination implying activation of this molecule.

The sulfur dioxide ligand also displays a variety of coordination geometries in transition metal complexes.<sup>52,53</sup> Those geometries which have been structurally characterized are shown in Figure 3. When associated with a single metal

Figure 3. Coordination Modes of Sulfur Dioxide  
with Transition Metals

Mode		Example	Reference
coplanar- $\eta^1$		$[\text{Ni}(\text{SO}_2)(\text{PPh}_3)_3]$ $[\text{CpRh}(\text{C}_2\text{H}_4)(\text{SO}_2)]$	54 55
pyramidal- $\eta^1$		$[\text{IrCl}(\text{CO})(\text{SO}_2)(\text{PPh}_3)_2]$ $[\text{RhCl}(\text{SO}_2)(\text{PPh}_3)_2]_2$	56 57
O,S- $\eta^2$		$[\text{Rh}(\text{NO})(\eta^2\text{-SO}_2)(\text{PPh}_3)_2]$ $[\text{RuCl}(\text{NO})(\eta^2\text{-SO}_2)(\text{PPh}_3)_2]$	58 59
bridging- $\mu_2$		$[\text{Ir}_2(\text{CO})_4\text{H}_2(\text{SO}_2)(\text{PPh}_3)_2]$ $[\text{Ir}_2(\text{CO})_2\text{I}_4(\text{SO}_2)(\text{PPh}_3)_2]$	60 61
$\eta^1\text{-O}$	M-O-S-O	$[\text{SbF}_5\text{OSO}]^a$	62

<sup>a</sup>Although Sb is not a transition metal, this represents a potential coordination mode in transition metal complexes.

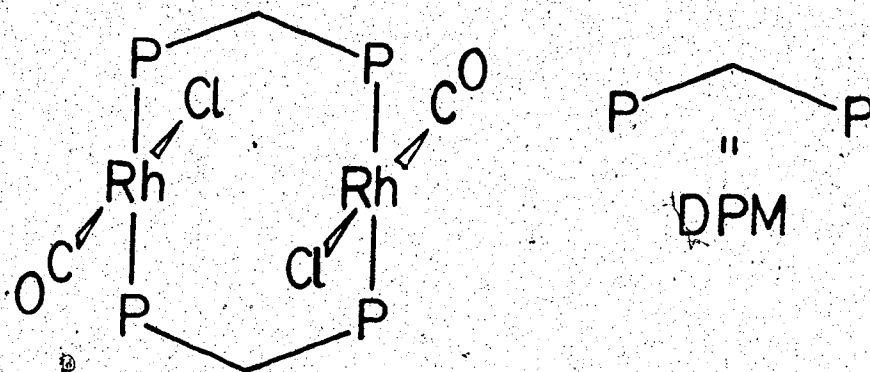
centre sulfur dioxide can exhibit the following coordination modes: the coplanar geometry, in which the M-SO<sub>2</sub> framework is approximately planar; the pyramidal geometry, with the SO<sub>2</sub> plane inclined to the M-S vector; O,S-η<sup>2</sup> coordination with the sulfur atom and one of the oxygen atoms coordinated to the metal in a side-on manner; and terminal η<sup>1</sup>-O coordination, in which the sulfur dioxide ligand is bound through one of the oxygen atoms. The coplanar and pyramidal coordination modes are often compared to the linear and bent geometries observed with the more extensively studied nitrosyl ligand.<sup>63</sup>

Sulfur dioxide has also been observed to bridge two metal centres in a symmetrical fashion. As now appears to be the case with the carbonyl ligand, a metal-metal bond is not a prerequisite to having a bridging SO<sub>2</sub> group. Therefore, in [(Cp)<sub>2</sub>Fe<sub>2</sub>(CO)<sub>4</sub>(μ-SO<sub>2</sub>)]<sup>64</sup> the SO<sub>2</sub> ligand is bridging and unsupported, whereas in [Ir<sub>2</sub>(CO)<sub>4</sub>H<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>(μ-SO<sub>2</sub>)]<sup>60</sup> the bridging SO<sub>2</sub> ligand is accompanied by a metal-metal bond. Sulfur dioxide coordination to a terminal halogen in a pyramidal fashion is also known, as for example in [Pt(Me)(I-SO<sub>2</sub>)(PPh<sub>3</sub>)<sub>2</sub>].<sup>65</sup>

Spectroscopic identification of the sulfur dioxide coordination mode is not without difficulty. Although the various coordination geometries have associated ranges of ν(SO), large regions of overlap exist, especially between the bridging and pyramidal modes where the regions

are essentially superimposed.<sup>53</sup> Thus unambiguous identification of the coordination geometry using infrared techniques, is in some cases difficult.

The chemistry of the above small molecules will be limited, in this thesis, to that involving binuclear diphosphine and diarsine bridged complexes of rhodium, similar to that shown below for *trans*-[RhCl(CO)(DPM)]<sub>2</sub>:<sup>66</sup>



These binuclear complexes are closely related to group VIII mononuclear, four coordinate phosphine complexes such as Vallarino's compound, [RhCl(CO)(PPh<sub>3</sub>)<sub>2</sub>]<sup>67</sup> and Vaska's compound, [IrCl(CO)(PPh<sub>3</sub>)<sub>2</sub>].<sup>68</sup> These mononuclear compounds have received a great deal of attention in the last twenty years and have been found to display a wide variety of small molecule addition and oxidative addition reactions.<sup>69,70</sup> The analogous binuclear complexes, of the type shown above, have on the other hand received much less attention and very little small molecule chemistry has been reported

for them. In these binuclear complexes the metal atoms are held in close proximity by the bridging DPM or DAM ligands and, although chemistry similar to the related mononuclear complexes might be expected, one might also anticipate differences in their chemistries owing to the effects of metal proximity, in the binuclear case. In these species, the metal centres can react independently of each other reacting essentially as two monomeric units, or one metal centre can perturb the other thereby altering its chemistry significantly relative to the related mononuclear complex. Balch and Tulyathan<sup>71</sup> have carried out studies in this regard, relating the chemistry at the metal centres to the distance between them, utilizing diphosphines and other bidentate ligands of varying bite size to bridge two square planar Rh(I) centres. In one example, involving complexes of the type  $[\text{RhCl}(\text{CO})(\text{L-L})]_2$ , where  $\text{L-L} = \text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2$  ( $n=3,4$ ),  $\text{SO}_2$  attack was observed at only one rhodium site. It was therefore concluded that the normal reactivity of the rhodium site is diminished in these dimeric complexes and it was suggested that this lack of reactivity resulted from the inability of the unreactive rhodium site to re-adjust its coordination geometry to the arrangement necessary to bind a second substrate molecule.

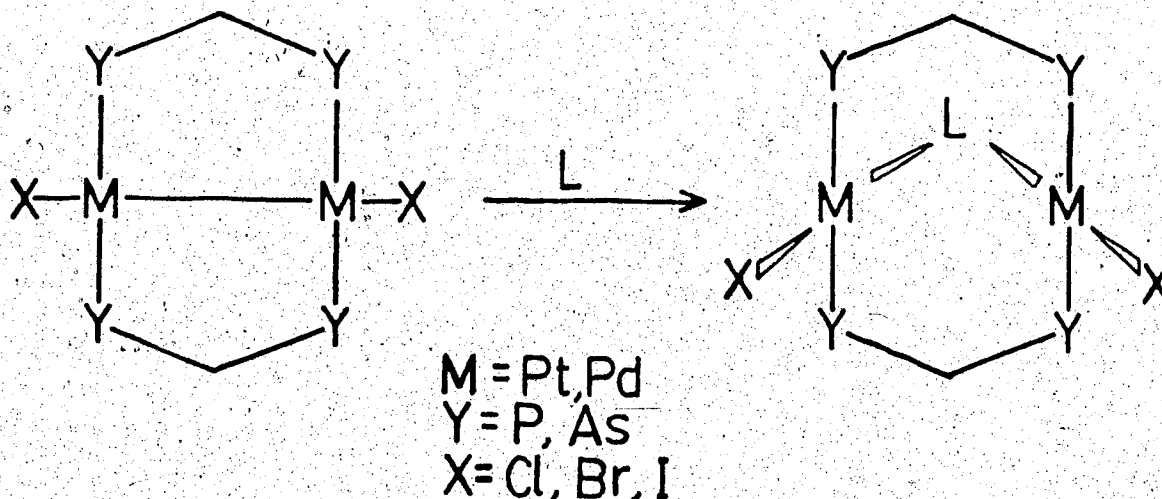
The close proximity of the metals in binuclear species also suggests that they may serve as useful models for multi-centered metal catalysis.<sup>11</sup>

Although binuclear transition metal species have been reported for several bidentate diphosphine and diarsine ligands including  $R_2PPR_2$  ( $R = Me, Et, Ph$ ),<sup>72</sup>  $Me_2AsAsMe_2$ ,<sup>73</sup>  $Me_2XYXMe_2$  ( $X = P, As; Y = O, S$ ),<sup>73,74</sup>  $Me_2P(CH_2)_2PMe_2$ ,<sup>75</sup>  $Ph_2P(CH_2)_2AsPh_2$ ,<sup>76</sup>  $(t-Bu)_2P(CH_2)_nP(t-Bu)_2$  ( $n = 10, 12$ ),<sup>77</sup>  $Ph_2PCC(PPh_2)(CF_2)_n$  ( $n = 2, 3, 4$ )<sup>78,79</sup> and  $Me_2AsCC(AsMe_2)(CF_2)_n$  ( $n = 2, 3$ ),<sup>78,79</sup> no reports on the chemistry of binuclear species containing these ligands with the small molecules of interest have appeared.

With the ligand of specific interest, bis(diphenylphosphino)methane (DPM) and bis(diphenylarsino)methane (DAM), several binuclear transition metal complexes are known, including:  $[Mn_2(CO)_8(DPM)]$ ,<sup>80</sup>  $[Mn_2(CO)_6(DPM)_2]$ ,<sup>80</sup>  $[Mn_2(CO)_4(\mu-CO)(DPM)_2]$ ,<sup>37,80</sup>  $[Mn_2(CO)_5(\textit{para-CH}_3C_6H_4NC)(DPM)_2]$ ,<sup>81</sup>  $[Mn(CO)_4(\mu\textit{-para-CH}_3C_6H_4NC)(DPM)_2]$ ,<sup>81</sup>  $[Fe_2(CO)_6(\mu-CO)(DPM)_2]$ <sup>33</sup> and  $[IrCl(CO)(DPM)]_2$ .<sup>82</sup> Again the reactivity of these complexes towards small molecules has not been reported.

Some small molecule chemistry has been reported for binuclear DPM and DAM species of Pt, Pd and Rh. The Pt(I)<sup>83</sup> and Pd(I)<sup>32,84</sup> species of the type  $[MX(L-L)]_2$  ( $M = Pd, Pt; X = Cl, Br; L-L = DPM, DAM$ ), for example, undergo facile reactions with several small molecules including CO,<sup>32,41,84</sup> SO<sub>2</sub>,<sup>85</sup> PhN<sub>2</sub>,<sup>86</sup> CNR ( $R = CH_3, C_6H_{11}, C_6H_5, \textit{para-CH}_3-C_6H_4$ ),<sup>84</sup> acetylenes,<sup>87</sup> olefins,<sup>87</sup> N<sub>2</sub>CH<sub>2</sub> (which yields a methylene species)<sup>88</sup> and S<sub>8</sub> (which yields a sulfido species)<sup>85b</sup> as

shown below, by inserting into the metal-metal bond.



The carbonyl adduct,  $[\text{Pd}_2\text{Cl}_2(\mu\text{-CO})(\text{DAM})_2]$ ,<sup>32</sup> represented the first structural characterization of a carbonyl ligand bridging two nonbonded metal centres. In addition, the insertions of CO and SO<sub>2</sub> in these systems were shown to be reversible. Kubiak and Eisenberg<sup>89</sup> have aptly dubbed these species "A-frame" complexes owing to the configuration of the equatorial ligands which roughly describes a letter A having the ligand L at the apex.

In addition, DPM-bridged Pd species are reported to undergo two other reactions. The first involves insertion of SnCl<sub>2</sub> into the Pd-Cl bonds of  $[\text{PdCl}(\text{DPM})]_2$  yielding  $[\text{Pd}_2\text{Cl}(\text{SnCl}_3)(\text{DPM})_2]$  and  $[\text{Pd}(\text{SnCl}_3)(\text{DPM})]_2$ .<sup>90</sup> The second involves halide displacement from  $[\text{Pd}_2\text{Cl}_2(\mu\text{-CNR})(\text{DPM})_2]$  in the presence of excess isocyanide to reversibly yield the dicationic species  $[\text{Pd}_2(\text{CNR})_2(\mu\text{-CNR})(\text{DPM})_2]^{2+}$ .<sup>84</sup>

Some small molecule chemistry of DPM-bridged rhodium complexes has also been reported. The reaction of the rhodium dicarbonyl "A-frame" species,  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]\text{-}[\text{BPh}_4]$  with CO produces the tricarbonyl complex  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$ .<sup>35,91</sup> However in contrast to the Pd and Pt species (vide supra) where insertion into a metal-metal bond occurs, carbon monoxide addition here occurs with the formation of a Rh-Rh bond. This tricarbonyl species verifies that small molecules can coordinate in the open bridging site of these "A-frame" complexes as was originally suggested by Eisenberg and Kubiak.<sup>89</sup> The analogous sulfido bridged "A-frame" species,  $[\text{Rh}_2(\text{CO})_2(\mu\text{-S})(\text{DPM})_2]$  has been treated with MeI, EtI, or LiI followed by CO addition resulting in a species postulated as  $[\text{RhI}(\text{CO})(\mu\text{-CO})(\text{DPM})]_2$ .<sup>89</sup> However, based on the spectral data presented, this species is probably more correctly assigned as an iodo-bridged tricarbonyl complex, analogous to the cationic chloro-bridged species noted above. In addition, the reaction of the sulfido-bridged complex with HCl yields the species *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$ .<sup>89</sup> Both  $[\text{Rh}_2(\text{CO})_2(\mu\text{-S})(\text{DPM})_2]$ <sup>89</sup> and *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$ <sup>71</sup> have been reported to react with SO<sub>2</sub>, however the formulations for the products are unknown. Finally *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  has been observed to react with iodine yielding the novel Rh(II) species  $[\text{RhClI}(\text{CO})(\text{DPM})]_2$ .<sup>71</sup>

Owing to the lack of small molecule chemistry with binuclear Rh species and because of the potential relevance of



such studies to catalytically interesting systems, as mentioned previously, an investigation into the chemistry of trans-[RhCl(CO)(DPM)]<sub>2</sub> and [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-Cl)(DPM)<sub>2</sub>]<sup>+</sup> with CO, CS<sub>2</sub> and SO<sub>2</sub> was undertaken.

Since it is difficult on the basis of analytical and spectral data to unambiguously assign the mode of small molecule coordination, the technique of X-ray diffraction was used extensively throughout this study. The reader is referred to several standard texts for detailed discussions of the theoretical and experimental considerations of X-ray diffraction. 92-95

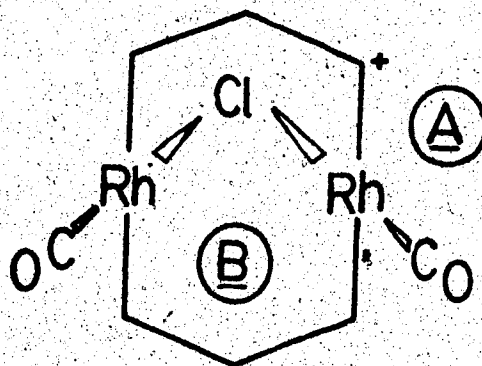
## CHAPTER II.

### The Structure of $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$ $[\text{BF}_4]^-$ :

#### A Binuclear "A-frame" Complex

#### INTRODUCTION

The cationic complex,  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  (1), was assumed to be an "A-frame" type species, as shown below, based on spectral data, on the structural characterization of its carbonyl adduct, <sup>35,91</sup>  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2]^+$  (2) and on analogies with the sulfido-bridged species, <sup>89</sup>  $[\text{Rh}_2(\text{CO})_2(\mu\text{-S})(\text{DPM})_2]$  (3).



1

Complex 1 reacts reversibly with  $\text{CO}$  <sup>35,91</sup> and  $\text{SO}_2$  <sup>96</sup> (see Chapter IV) and undergoes facile reactions with several other small molecules, including  $\text{NO}$  <sup>97</sup> and tetracyanoethylene. <sup>98</sup> The reactions of 1 with  $\text{CO}$  and  $\text{SO}_2$  contrast the two possible modes of attack on this species by small molecules.

Whereas CO attacks the open terminal coordination site A, remote from the bridging site B and results in one of the originally coordinated carbonyl ligands swinging into the bridging site;<sup>91</sup> SO<sub>2</sub> seems to attack directly at the bridging site yielding  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\mu\text{-SO}_2)(\text{DPM})_2]^+$ .<sup>96</sup>

The structural determination of the closely related, sulfido bridged "A-frame" complex 3,<sup>89</sup> indicated that the bridging site was blocked, at least in the solid state, by four of the DPM phenyl groups. In particular, two rings were found to severely obstruct this site. Although the details of the chemistry of 3 with small molecules are not known to us, other "A-frame" species; having their bridging sites obstructed in the same way, show chemistry consistent with terminal ligand attack as opposed to attack at the bridging site (see Chapter IV). Since 1 seems to allow attack at both the bridging and terminal sites, it was of interest to obtain precise structural information on this "A-frame" species with hopes of establishing possible structure-reactivity correlations.

### EXPERIMENTAL

All solvents used throughout this study were dried and degassed prior to use and all reactions were performed under Schlenk conditions using an atmosphere of dinitrogen or the reactant gas. RhCl<sub>3</sub>·3H<sub>2</sub>O was purchased from Research Organic/Inorganic Chemical Corporation and DPM and

DAM were purchased from Strem Chemicals. All other chemicals were reagent grade and used as received. Infrared spectra were recorded on either a Perkin Elmer Model 467 spectrometer or a Nicolet 7199 F.T. interferometer using Nujol mulls on KBr plates. NMR spectra were recorded on a Bruker HFX-90 NMR spectrometer. Conductivity measurements were obtained on a Yellow Springs Instruments Model 31 Conductivity bridge using approximately 1.0 mM solutions in acetone.

Preparation of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$

Treatment of a solution of 0.100 g (0.202 mmol) of  $[\text{RhCl}(\text{COD})]_2^{99}$  in 20 mL of  $\text{CH}_2\text{Cl}_2$  with 0.103 g (0.269 mmol) of DPM dissolved in 5 mL of toluene under a carbon monoxide atmosphere yielded  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{RhCl}_2(\text{CO})_2]$ . Addition of 0.458 g (1.34 mmol) of  $\text{NaBPh}_4$ , followed by 40 mL of  $\text{Et}_2\text{O}$  resulted in the precipitation of the cationic tricarbonyl species as the  $\text{BPh}_4^-$  salt in 90% yield. Slow concentration of this solution of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$  under a dinitrogen flow yielded the dicarbonyl species,  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$ , as a yellow-orange microcrystalline solid.

The serendipitous crystallization of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$

To a solution of 0.100 g (0.072 mmol) of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$  in 8 mL of acetone was added 0.020 g (0.080 mmol) of  $[\text{PhN}_2][\text{PF}_6]$ . Slow diffusion of  $\text{Et}_2\text{O}$  into the reaction mixture yielded yellow-orange prismatic crys-

tals. Although too few of the yellow-orange crystals were obtained for elemental analysis or a  $^{31}\text{P}$  NMR spectrum, an infrared spectrum of the complex ( $\nu(\text{CO})$  1995(s), 1978(vs)  $\text{cm}^{-1}$ ;  $\nu(\text{BF})$  1060 (m,br)  $\text{cm}^{-1}$ ) indicated that they were  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$ .

#### Preparation of $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$

To a solution of 0.100 g (0.075 mmol) of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{RhCl}_2(\text{CO})_2]$  in 10 mL of  $\text{CH}_2\text{Cl}_2$  was added 0.017 g (0.150 mmol) of  $\text{NaBF}_4$ . Slow concentration of this solution under a dinitrogen stream yielded yellow-orange crystals of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$ . The infrared spectrum of this compound was identical to that of the crystals initially obtained, one of which was used in the structure determination (vide infra).

#### $^{31}\text{P}$ and $^{19}\text{F}$ NMR Results

A solution was prepared in  $d^6$ -acetone containing 0.050 g (0.036 mmol) of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$  and 0.010 g (0.040 mmol) of  $[\text{PhN}_2][\text{PF}_6]$ . The  $^{19}\text{F}$  and  $^{31}\text{P}\{^1\text{H}\}$  NMR were recorded immediately after preparation and again after approximately two weeks. The initial spectra showed that the only fluorine containing species was the  $\text{PF}_6^-$  anion ( $^{19}\text{F}$  NMR  $\delta = 71.7$  ppm,  $^{100}$  doublet,  $|J_{\text{P-F}}| = 707$  Hz;  $^{31}\text{P}\{^1\text{H}\}$  NMR  $\delta = 144.0$  ppm,  $^{101}$  septet,  $J_{\text{P-F}} = 708$  Hz). The spectra of the aged sample showed the presence of the  $\text{PF}_6^-$  anion as well as resonances in the  $^{19}\text{F}$  NMR at  $\delta = 130.8$  ppm

(heptet,  $|J_{F-H}| = 6.3$  Hz, possibly  $\text{Me}_2\text{SiF}_2$ );  $\delta = 150.0$  ppm (singlet) and  $\delta = 150.1$  ppm (br singlet,  $\text{BF}_4^-$ ). In both  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra (new and two week old samples) the resonance due to the cation  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  was observed. No other rhodium-DPM species was detected.

### Data Collection

A crystal of the title compound was mounted and sealed in a glass capillary. Preliminary film data showed  $\bar{1}$  Laue symmetry and no systematic absences, consistent with the space groups  $P1$  and  $P\bar{1}$ . The centrosymmetric space group  $P\bar{1}$  was chosen and later verified by; (1) the successful refinement of the structure with acceptable positional parameters, thermal parameters and agreement indices, and (2) the location of all hydrogen atoms in electron density difference maps. Accurate cell parameters were obtained by a least-squares analysis of the setting angles of 12 carefully centered reflections chosen from diverse regions of reciprocal space ( $50^\circ < 2\theta < 70^\circ$ ,  $\text{CuK}\alpha$  radiation) and obtained by using a narrow X-ray source (see Table I for pertinent crystal data). A cell reduction<sup>102</sup> failed to show the presence of higher symmetry. The reduced cell is reported.

Intensity data were collected on a Picker four-circle automated diffractometer equipped with a scintillation counter and pulse-height analyzer, tuned to accept 90% of the  $\text{CuK}\alpha$  peak. Background counts were measured at both ends of the scan range with crystal and counter stationary.

Table 1. Summary of Crystal Data and Intensity Collection  
for  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$

Compound	$[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$																																												
Formula	$\text{C}_{52}\text{H}_{44}\text{B}_1\text{Cl}_1\text{F}_4\text{O}_2\text{P}_4\text{Rh}_2$																																												
Formula Weight	1152.89 amu																																												
Reduced Cell Parameters																																													
a	13.044 (1) Å																																												
b	14.962 (1) Å																																												
c	12.800 (1) Å																																												
$\alpha$	96.20 (1) °																																												
$\beta$	92.56 (1) °																																												
$\gamma$	86.42 (1) °																																												
V	2476.8 Å <sup>3</sup>																																												
Z	2																																												
Density	1.545 g·cm <sup>-3</sup> (calc'd.) 1.547(5) g·cm <sup>-3</sup> (expt'l. by flotation)																																												
Space Group	$C_i^1 - P\bar{1}$																																												
Crystal Dimensions	0.345 x 0.303 x 0.147 mm																																												
Crystal Volume	0.0129 mm <sup>3</sup>																																												
Crystal Faces (and distances from an arbitrary origin within the crystal (mm))	<table border="0"> <tbody> <tr><td>1</td><td>1</td><td>0</td><td>(0.145)</td></tr> <tr><td>1</td><td><math>\bar{1}</math></td><td>0</td><td>(0.145)</td></tr> <tr><td><math>\bar{1}</math></td><td>1</td><td>0</td><td>(0.155)</td></tr> <tr><td><math>\bar{1}</math></td><td><math>\bar{1}</math></td><td>0</td><td>(0.195)</td></tr> <tr><td>0</td><td>0</td><td>1</td><td>(0.075)</td></tr> <tr><td>0</td><td>0</td><td><math>\bar{1}</math></td><td>(0.071)</td></tr> <tr><td>0</td><td><math>\bar{1}</math></td><td>0</td><td>(0.222)</td></tr> <tr><td>0</td><td>1</td><td><math>\bar{1}</math></td><td>(0.122)</td></tr> <tr><td>0</td><td><math>\bar{1}</math></td><td>1</td><td>(0.162)</td></tr> <tr><td><math>\bar{1}</math></td><td>0</td><td>1</td><td>(0.122)</td></tr> <tr><td><math>\bar{1}</math></td><td>0</td><td>0</td><td>(0.208)</td></tr> </tbody> </table>	1	1	0	(0.145)	1	$\bar{1}$	0	(0.145)	$\bar{1}$	1	0	(0.155)	$\bar{1}$	$\bar{1}$	0	(0.195)	0	0	1	(0.075)	0	0	$\bar{1}$	(0.071)	0	$\bar{1}$	0	(0.222)	0	1	$\bar{1}$	(0.122)	0	$\bar{1}$	1	(0.162)	$\bar{1}$	0	1	(0.122)	$\bar{1}$	0	0	(0.208)
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0	0	1	(0.075)																																										
0	0	$\bar{1}$	(0.071)																																										
0	$\bar{1}$	0	(0.222)																																										
0	1	$\bar{1}$	(0.122)																																										
0	$\bar{1}$	1	(0.162)																																										
$\bar{1}$	0	1	(0.122)																																										
$\bar{1}$	0	0	(0.208)																																										
Temperature	20°C																																												
Radiation	$\text{CuK}\alpha$ ( $\lambda=1.540562$ Å) filtered with 0.5 mil thick nickel foil																																												
$\mu$	77.256 cm <sup>-1</sup>																																												
Range in Absorption Correction Factors	0.156 - 0.403																																												

Table 1, continued

Takeoff Angle	2.90°
Scan Speed	2° in 2θ/min
Scan Range	0.80° below $K_{\alpha 1}$ to 0.80° above $K_{\alpha 2}$
Background Counting Time	10s ( $3^\circ < 2\theta < 75^\circ$ ); 20s ( $75^\circ < 2\theta < 104^\circ$ ); 40s ( $104^\circ < 2\theta < 120^\circ$ )
2θ limits	$3^\circ < 2\theta < 120^\circ$
2θ units for centred reflections	$50^\circ < 2\theta < 70^\circ$
Final number of variables	298
Unique Data Collected	7416
Unique Data Used ( $F_o^2 \geq 3\sigma(F_o^2)$ )	5729
Error in observation of unit weight	1.792
R	0.046
$R_w$	0.064



Assuming approximate linearity of background, the intensity of the peak (I) is given by:

$$I = PK - (B_1 + B_2) t_p / t_B \quad (2)$$

where PK = peak count,  $t_p$  = peak scan time,  $t_B$  = the sum of the two background collection times and  $B_1$  and  $B_2$  are the background counts. Standard deviations in the intensity were computed from the relationship:

$$\sigma(I) = (PK + t^2 B_T + p^2 I^2)^{1/2} \quad (3)$$

where  $B_T = B_1 + B_2$ ,  $t = t_p / t_B$  and  $p$  is an ignorance factor used to account for machine uncertainty and to prevent unreasonably high weighting being applied to reflections of high intensity (a value of 0.05 was used for  $p$ ).<sup>103</sup> The intensities of three standard reflections were measured automatically every 100 reflections and four additional standards were measured three times a day in order to check crystal stability and centering. All standards remained constant to within 1.5% of the mean throughout the data collection.

The intensities of 7416 unique reflections ( $3^\circ \leq 2\theta \leq 120^\circ$ ) were measured using CuK $\alpha$  radiation. Of these, 5729 were considered significantly above background ( $F^2 / \sigma(F^2) \geq 3.0$ , see Table 1) and were used in subsequent calculations. These observed data were reduced to structure factor amplitudes and standard deviations in the structure factors,  $\sigma(F)$ , by correction for Lorentz, polarization and absorption

effects.<sup>92-95</sup> Similar procedures of data collection and reduction were followed on all subsequent structures.

### Structure Solution and Refinement

A Patterson map<sup>104,105</sup> was computed between the limits  $0 \leq u \leq 1.0$ ,  $0 \leq v \leq 1.0$  and  $0 \leq w \leq 0.5$ . The Rh-Rh vectors are derived for two independent rhodium atoms in the space group  $P\bar{1}$  in Table 2. The origin peak corresponds to the sum of the vectors between every atom and itself, in the unit cell. Therefore the magnitude of the origin vector is roughly proportional to:  $\sum_i z_i^2$ , summed over the contents of the unit cell, =  $(4 \times 45^2 + 2 \times 17^2 + 8 \times 15^2 + 8 \times 9^2 + 4 \times 8^2 + 104 \times 6^2 + 2 \times 5^2 + 88 \times 1^2) = 15264$ . In the Fourier program used to calculate the vector map, the origin peak is normalized to 1000. Therefore assuming comparable thermal parameters for all atoms one expects the Rh(1)-Rh(2) vectors which are doubly weighted (see Table 2) to have an approximate, normalized value of 265 (ie.  $\frac{2 \times 45^2}{15264} \times 1000$ ), and the Rh(1)-Rh(1) and Rh(2)-Rh(2) vectors, which are singly weighted to have an intensity of 133 above background. Viewing the Patterson map, the nine most intense peaks of which, are summarized in Table 3, it is obvious that three vectors, instead of the anticipated two, are observed with weights comparable to those expected for the Rh(1)-Rh(2) vectors. One of these three, the second peak listed, is actually a result of Rh-P<sub>o</sub> vector build-up. Generally the DPM ligands are mutually trans

Table 2. Derivation of the Rh-Rh Vectors for the Space Group P1

	$x_1, y_1, z_1^a$	$\bar{x}_1, \bar{y}_1, \bar{z}_1$	$x_2, y_2, z_2$	$\bar{x}_2, \bar{y}_2, \bar{z}_2$
$x_1, y_1, z_1$	0, 0, 0	$2\bar{x}_1, 2\bar{y}_1, 2\bar{z}_1$	$-(x_1-x_2)$ $-(y_1-y_2)$ $-(z_1-z_2)$	$-(x_1+x_2)$ $-(y_1+y_2)$ $-(z_1+z_2)$
$\bar{x}_1, \bar{y}_1, \bar{z}_1$	$2x_1, 2y_1, 2z_1$	0, 0, 0	$x_1+x_2$ $y_1+y_2$ $z_1+z_2$	$x_1-x_2$ $y_1-y_2$ $z_1-z_2$
$x_2, y_2, z_2$	$x_1-x_2$ $y_1-y_2$ $z_1-z_2$	$-(x_1+x_2)$ $-(y_1+y_2)$ $-(z_1+z_2)$	0, 0, 0	$2\bar{x}_2, 2\bar{y}_2, 2\bar{z}_2$
$\bar{x}_2, \bar{y}_2, \bar{z}_2$	$x_1+x_2$ $y_1+y_2$ $z_1+z_2$	$-(x_1-x_2)$ $-(y_1-y_2)$ $-(z_1-z_2)$	$2x_2, 2y_2, 2z_2$	0, 0, 0

Vector Weight

0, 0, 0 4

$x_1+x_2, y_1+y_2, z_1+z_2$  2

$-(x_1+x_2), -(y_1+y_2), -(z_1+z_2)$  2

$x_1-x_2, y_1-y_2, z_1-z_2$  2

$-(x_1-x_2), -(y_1-y_2), -(z_1-z_2)$  2

$2x_1, 2y_1, 2z_1$  1

$2\bar{x}_1, 2\bar{y}_1, 2\bar{z}_1$  1

$2x_2, 2y_2, 2z_2$  1

$2\bar{x}_2, 2\bar{y}_2, 2\bar{z}_2$  1

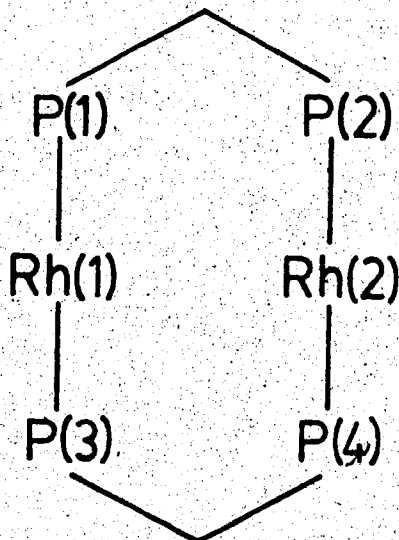
<sup>a</sup> $(x_1, y_1, z_1)$  and  $(x_2, y_2, z_2)$  are the coordinates of Rh(1) and Rh(2) respectively.

Table 3: Assignment of the Most Intense Patterson

## Map Vectors

No.	u	v	w	Relative Weight	Assignment
1	0.640	0.420	0.192	357	$(x_1+x_2, y_1+y_2, z_1+z_2)$
2	0.960	0.030	0.192	339	Rh-P vector build-up
3	0.160	0.120	0.064	290	$(x_1-x_2, y_1-y_2, z_1-z_2)$
4	0.120	0.150	0.224	190	Rh-P vector build-up
5	0.680	0.390	0.032	187	Rh-P vector build-up
6	0.800	0.540	0.256	180	$(2x_1, 2y_1, 2z_1)$
7	0.600	0.420	0.384	175	Rh-P vector build-up
8	0.000	0.180	0.000	152	Rh(1)-C1 and Rh(1)-O
9	0.480	0.270	0.160	148	$(2x_2, 2y_2, 2z_2)$

and the Rh-P framework is approximately planar as shown below:



The Rh(1)-P(1), Rh(2)-P(2), P(3)-Rh(1) and P(4)-Rh(2) vectors are therefore almost coincident, yielding a Rh-P vector build-up of approximate weight  $353 \left( \frac{2 \times 4 \times 15 \times 45}{15264} \times 1000 \right)$ . Similarly other vector build-ups may also occur. This complication in solving the Patterson maps continued throughout this study, however it is readily overcome by using image seeking techniques and comparing vector lengths. Typically Rh-P vectors are *ca.*  $2.35 \text{ \AA}$  whereas the Rh(1)-Rh(2) vectors are in the range  $2.7 - 3.4 \text{ \AA}$ . Applying these methods it became obvious that the first peak was associated with the Rh(1)-Rh(2) vector,  $(x_1+x_2, y_1+y_2, z_1+z_2)$  and the third peak with the Rh(1)-Rh(2) vector  $(x_1-x_2, y_1-y_2, z_1-z_2)$  with the latter having a distance from the origin of *ca.*  $2.87 \text{ \AA}$  (the approximate metal-metal separation in the

dimer). The second peak which is approximately 2.52 Å from the (1.0,0.0,0.0) origin is due to Rh-P vector build-up. The positions of the rhodium atoms are then calculated as Rh(1) (0.40,0.27,0.13) and Rh(2) (0.23,0.14,0.07). The sixth peak then corresponds to the  $(2x_1, 2y_1, 2z_1)$  vector and the ninth peak to the  $(2x_2, 2y_2, 2z_2)$  vector, with the intervening peaks resulting from vector build-up as indicated in Table 3.

A full-matrix, least-squares refinement based on the two rhodium atom positions converged in two cycles to  $R=0.46$  and  $R_w=0.56$ . These  $R$  factors as calculated in the least-squares program are defined as:

$$R = \frac{\sum ||F_O| - |F_C||}{\sum |F_O|} \quad (4)$$

and

$$R_w = \left\{ \frac{\sum w (|F_O| - |F_C|)^2}{\sum w |F_O|^2} \right\}^{1/2} \quad (5)$$

where  $|F_O|$  and  $|F_C|$  are the observed and calculated structure amplitudes, respectively, and  $w$ , the weighting factor, is defined as  $w = 1/\sigma^2(F)$ . The function minimized during the least square refinement was  $\sum w (|F_O| - |F_C|)^2$ . Structure factors were calculated using the atomic scattering factors taken from Cromer and Waber's<sup>106</sup> tabulation for all atoms except hydrogen for which the values of Stewart *et al.*<sup>107</sup> were used. Anomalous dispersion corrections,<sup>108</sup> both real and imaginary<sup>109</sup> were applied to  $F_C$ .

An electron density difference map, phased on the two rhodium atom positions, yielded the location of the phosphorus and chlorine atoms. A subsequent least-squares refinement of the electron density difference map calculated using the rhodium, phosphorus and chlorine atom positions, revealed the location of all other non-hydrogen atoms within the cation. The carbon atoms of the phenyl rings were refined in all least-squares calculations as rigid groups having mirror symmetry and C-C distances of 1.392 Å.

Although the infrared spectrum indicated that the present complex had crystallized as the  $\text{BF}_4^-$  salt, our initial unwillingness to accept the apparent transformation of  $\text{PF}_6^-$  and  $\text{BPh}_4^-$  into  $\text{BF}_4^-$  together with the pseudo octahedral coordination about the central atom in the electron density difference map, led us to attempt refinement of the electron density about the 1(c) and 1(f) inversion centres as  $\text{PF}_6^-$  anions. However, these refinement attempts proved unsuccessful, even considering disorder of the groups. The thermal parameters for both phosphorus atoms exceeded  $30 \text{ \AA}^2$  and chemically unreasonable P-F distances resulted. A closer inspection of the electron density difference map revealed that there were eight peaks about both sets of inversion centres and not just the six originally located. The placement of these eight peaks corresponded to superimposed, inversion related, tetrahedral  $\text{BF}_4^-$  groups. Furthermore, the central peaks were more consistent with boron than phosphorus, having intensities in the electron density dif-

ference map (4.7 and 3.3 e/Å<sup>3</sup>) comparable to the half-weighted fluorine peaks (3.7-1.8 e/Å<sup>3</sup>). Refinement of this model as inversion disordered BF<sub>4</sub><sup>-</sup> groups proceeded well, resulting in reasonable bond lengths, thermal parameters and well defined tetrahedral geometries about the central boron atom.

The data were corrected for the effects of absorption by Gaussian integration. All non-group atoms excluding hydrogen were refined with anisotropic thermal parameters, where the form of the thermal ellipsoid used was  $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$ .

An electron density difference map at this stage revealed the location of all hydrogen atoms in the structure. These atoms were included as fixed contributions in calculating the structure factors and were not refined. Their idealized positions were calculated from the geometries of their attached carbon atoms by using C-H distances of 0.95 Å. Hydrogen atoms were assigned isotropic thermal parameters of 1 Å<sup>2</sup> greater than those of their attached carbon atom or 1 Å<sup>2</sup> greater than the equivalent isotropic B when the carbon atom was refined anisotropically. Throughout this study hydrogen atoms were always handled in a similar manner.

The final model with 298 parameters varied converged to  $R = 0.046$  and  $R_w = 0.064$ . In the final electron density difference map all of the highest 20 peaks were in the vicinity of the phenyl rings (0.66-0.41 e/Å<sup>3</sup>), with smaller



residuals in the areas of the  $\text{BF}_4^-$  anions. A typical carbon atom on an earlier difference map had an electron density of about  $5.0 \text{ e}/\text{\AA}^3$ .

The programs used in the solution and refinement of structure and presentation of data are listed briefly in Appendix I.

### Results

The final positional and thermal parameters for the nongroup and group atoms are given in Tables 4 and 5, respectively. The idealized positional and thermal parameters for the hydrogen atoms are given in Table 6. Least-squares plane calculations are recorded in Table 7 and selected bond lengths and angles are shown in Tables 8 and 9, respectively. A listing of the observed and calculated structure amplitudes is available.<sup>110</sup>

The unit cell of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$  is shown in Figure 4. The crystallographic  $b$  axis is horizontal to the right, the  $c$  axis runs from top to bottom and the  $a$  axis goes into the page. With the exception of the methylene hydrogen atoms, which are drawn artificially small for clarity of the drawing, 20% thermal ellipsoids are used on this and all subsequent drawings unless noted otherwise. Only one set of the inversion disordered F atoms for each  $\text{BF}_4^-$  group is included. Figure 5 presents a perspective view of the  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  cation, including the numbering scheme. The numbering of the phenyl carbon atoms

starts at the carbon bound to the phosphorus atom and increases sequentially around the ring. The inner coordination sphere of the  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  cation is shown in Figure 6 along with some relevant bond lengths. In this figure 50% thermal ellipsoids are used. The two independent tetrafluoroborate anions are shown in Figure 7; again only one of each of the disorder sets of F atoms is included.

TABLE 4. Positional and Thermal Parameters For The Nongroup Atoms of [Rh2(CO)2(mu-C1)(DPM)2][BF4].

Atom	x	y	z	U11	U22	U33	U12	U13	U23
Rh(1)	0.40834(4)	0.26969(3)	0.12814(3)	4.39(3)	3.55(3)	2.97(2)	-0.60(2)	0.40(2)	0.16(2)
Rh(2)	0.22996(3)	0.13772(3)	0.07315(3)	3.50(3)	4.48(3)	2.83(2)	-0.32(2)	0.20(2)	0.02(2)
C1	0.4043(1)	0.1092(1)	0.1290(1)	4.06(8)	3.84(8)	4.00(7)	0.05(6)	-0.07(6)	0.38(6)
P(1)	0.3539(1)	0.2916(1)	0.2999(1)	4.30(9)	3.56(8)	2.98(7)	-0.28(7)	0.24(6)	0.20(6)
P(2)	0.1866(1)	0.1546(1)	0.2482(1)	3.84(8)	3.97(9)	3.02(7)	-0.31(7)	0.19(6)	0.37(6)
P(3)	0.4513(1)	0.2486(1)	-0.0471(1)	3.76(8)	4.04(9)	3.41(8)	-0.14(7)	0.54(6)	0.41(7)
P(4)	0.2816(1)	0.1132(1)	-0.0994(1)	3.56(8)	4.34(9)	3.03(7)	-0.08(7)	0.31(6)	-0.02(6)
O(1)	0.4525(5)	0.4614(4)	0.1349(5)	12.0(5)	4.9(3)	7.0(4)	-2.7(3)	1.0(4)	0.4(3)
O(2)	0.0117(4)	0.1436(5)	0.0009(5)	3.8(3)	16.0(7)	6.7(4)	-0.9(3)	-0.5(3)	0.4(4)
C(1)	0.4330(6)	0.3875(5)	0.1318(5)	6.8(5)	4.8(4)	3.5(3)	-1.4(4)	1.0(3)	-0.2(3)
C(2)	0.0969(6)	0.1438(6)	0.0295(5)	4.6(4)	9.5(6)	3.1(3)	-0.5(4)	1.1(3)	0.1(4)
C(3)	0.2926(5)	0.1943(4)	0.3379(4)	4.3(3)	3.3(3)	2.7(3)	-0.6(3)	0.2(3)	0.3(2)
C(4)	0.4151(5)	0.1398(4)	-0.1155(5)	3.9(3)	4.4(4)	3.1(3)	-0.5(3)	0.4(3)	0.1(3)
B(1)	1/2	0	1/2	8(1)	6(1)	24(4)	1(1)	-5(2)	5(2)
B(2)	1/2	0.0401(7)	0	5.5(8)	8(1)	4.4(6)	-3.8(7)	1.8(6)	-1.4(6)
F(1)	0.4693(8)	-0.0482(9)	0.400(1)	7.8(7)	7.0(7)	16(1)	1.2(6)	0.5(8)	3.8(7)
F(2)	0.416(1)	-0.057(2)	0.518(1)	11(1)	9.2(9)	15(1)	-0.1(8)	-1.5(9)	4.1(8)
F(3)	0.585(1)	0.071(2)	0.471(2)	7.4(9)	20(2)	25(2)	1(1)	-2(1)	10(2)
F(4)	0.504(3)	0.516(2)	0.590(2)	26(3)	34(4)	26(4)	-11(3)	-8(3)	21(3)
F(5)	-0.021(3)	0.516(2)	0.101(1)	17(2)	21(2)	7(1)	4(2)	2(1)	1(1)
F(6)	-0.101(1)	0.543(2)	-0.036(1)	10(1)	28(2)	10(1)	4(1)	-0.3(9)	2(1)
F(7)	-0.015(3)	0.420(2)	-0.032(3)	24(3)	30(3)	22(3)	-13(3)	11(2)	-11(3)
F(8)	0.062(2)	0.536(4)	-0.036(4)	14(2)	40(5)	23(3)	-11(3)	5(3)	8(4)

<sup>a</sup> Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

<sup>b</sup> The form of the thermal ellipsoid is:  $\exp[-2\pi i(xa + yb + zc)]$ . The quantities given in the table are the thermal coefficients  $\times 10^4$ .

TABLE 5. Derived Parameters For the Rigid Group Atoms of  $[\text{Rh}_2(\text{CO})_2(\text{mu}_3\text{-C})](\text{DPM})_2[\text{BF}_4]$ .

Atom	X	Y	Z	B(A <sup>1</sup> )	Atom	X	Y	Z	B(A <sup>1</sup> )
C(11)	0.4583(4)	0.3097(3)	0.3990(3)	3.2(1)	G(51)	0.3953(4)	0.3319(3)	-0.1297(5)	3.1(1)
C(12)	0.5109(4)	0.3878(3)	0.3988(4)	5.1(2)	C(52)	0.3195(4)	0.3956(3)	-0.0927(3)	3.7(1)
C(13)	0.5950(4)	0.4031(3)	0.4678(4)	6.1(2)	C(53)	0.2792(3)	0.4598(3)	-0.1566(4)	4.7(2)
C(14)	0.6266(4)	0.3403(3)	0.5370(3)	5.2(2)	C(54)	0.3146(4)	0.4603(3)	-0.2575(5)	4.8(2)
C(15)	0.5740(4)	0.2622(3)	0.5373(4)	4.7(2)	C(55)	0.3904(4)	0.3966(3)	-0.2945(3)	4.9(2)
C(16)	0.4899(4)	0.2469(3)	0.4683(4)	4.0(1)	C(56)	0.4308(3)	0.3324(3)	-0.2306(4)	4.1(1)
C(21)	0.2626(4)	0.3859(3)	0.3369(5)	3.1(1)	C(61)	0.5878(3)	0.2488(4)	-0.0706(3)	3.4(1)
C(22)	0.2289(4)	0.3976(3)	0.4394(5)	4.0(1)	C(62)	0.6338(4)	0.3306(3)	-0.0484(4)	5.0(2)
C(23)	0.1575(5)	0.4677(3)	0.4696(3)	4.9(2)	C(63)	0.7376(4)	0.3360(3)	-0.0662(4)	5.8(2)
C(24)	0.1199(4)	0.5260(3)	0.3974(5)	5.3(2)	C(64)	0.7955(3)	0.2596(4)	-0.1063(3)	5.3(2)
C(25)	0.1537(4)	0.5143(3)	0.2949(5)	5.4(2)	C(65)	0.7495(4)	0.1778(3)	-0.1285(4)	7.5(2)
C(26)	0.2251(5)	0.4443(3)	0.2647(3)	4.4(1)	C(66)	0.6457(4)	0.1725(3)	-0.1106(4)	5.5(2)
C(31)	0.1580(4)	0.0486(3)	0.2949(4)	3.1(1)	C(71)	0.2819(4)	-0.0054(3)	-0.1488(5)	3.6(1)
C(32)	0.0703(4)	0.0085(3)	0.2508(4)	4.7(2)	C(72)	0.3512(4)	-0.0443(3)	-0.2225(3)	4.9(2)
C(33)	0.0407(3)	-0.0706(3)	0.2858(3)	5.5(2)	C(73)	0.3497(4)	-0.1357(4)	-0.2571(3)	6.4(2)
C(34)	0.0986(4)	-0.1097(3)	0.3647(4)	6.7(2)	C(74)	0.2789(4)	-0.1882(3)	-0.2780(5)	6.4(2)
C(35)	0.1862(4)	-0.0696(3)	0.4087(4)	6.5(2)	C(75)	0.2096(4)	-0.1493(3)	-0.1443(3)	6.9(2)
C(36)	0.2159(3)	0.0095(3)	0.3738(3)	4.6(2)	C(76)	0.2110(4)	-0.0579(4)	-0.1097(3)	5.3(2)
C(41)	0.0735(5)	0.2272(3)	0.2846(3)	3.2(1)	C(81)	0.2112(4)	0.1735(3)	-0.1989(3)	3.2(1)
C(42)	-0.0436(4)	0.2979(3)	0.2256(3)	4.2(1)	C(82)	0.2215(4)	0.1442(3)	-0.3051(5)	4.5(1)
C(43)	-0.1006(5)	0.3531(3)	0.2515(5)	5.2(2)	C(83)	0.1700(5)	0.1919(3)	-0.3811(3)	5.5(2)
C(44)	-0.0705(6)	0.3375(3)	0.3364(3)	5.4(2)	C(84)	0.1082(4)	0.2687(3)	-0.3509(3)	5.5(2)
C(45)	0.0165(4)	0.2668(3)	0.3954(3)	5.0(2)	C(85)	0.0979(4)	0.2979(3)	-0.2447(5)	5.2(2)
C(46)	0.0165(4)	0.2116(3)	0.3695(5)	4.0(1)	C(86)	0.1494(5)	0.2503(3)	-0.1687(3)	4.1(1)

## Rigid Group Parameters

	X <sup>a</sup>	Y <sup>c</sup>	Z <sup>c</sup>	Delta <sup>b</sup>	Epsilon	Eta
Ring1	0.5425(2)	0.3250(2)	0.4680(3)	0.449(3)	2.401(3)	6.049(3)
Ring2	0.1913(2)	0.4560(2)	0.3671(3)	2.443(3)	1.338(4)	1.187(4)
Ring3	0.1283(3)	-0.0306(2)	0.3298(3)	3.671(3)	2.445(4)	4.772(3)
Ring4	-0.0135(2)	0.2823(2)	0.3105(2)	-0.699(3)	0.826(4)	5.497(4)
Ring5	0.3550(2)	0.3961(2)	-0.1936(2)	2.424(3)	1.212(4)	2.062(3)
Ring6	0.6916(3)	0.2542(3)	-0.0884(3)	3.350(4)	0.241(3)	3.025(3)
Ring7	0.2804(3)	-0.0968(2)	-0.1834(3)	3.311(3)	0.726(4)	4.582(3)
Ring8	0.1597(2)	0.2211(2)	-0.2749(3)	-0.653(3)	1.719(4)	3.792(3)

<sup>a</sup><sup>b</sup><sup>c</sup><sup>d</sup><sup>e</sup><sup>f</sup><sup>g</sup><sup>h</sup><sup>i</sup><sup>j</sup><sup>k</sup><sup>l</sup><sup>m</sup><sup>n</sup><sup>o</sup><sup>p</sup><sup>q</sup><sup>r</sup><sup>s</sup><sup>t</sup><sup>u</sup><sup>v</sup><sup>w</sup><sup>x</sup><sup>y</sup><sup>z</sup><sup>aa</sup><sup>ab</sup><sup>ac</sup><sup>ad</sup><sup>ae</sup><sup>af</sup><sup>ag</sup><sup>ah</sup><sup>ai</sup><sup>aj</sup><sup>ak</sup><sup>al</sup><sup>am</sup><sup>an</sup><sup>ao</sup><sup>ap</sup><sup>aq</sup><sup>ar</sup><sup>as</sup><sup>at</sup><sup>au</sup><sup>av</sup><sup>aw</sup><sup>ax</sup><sup>ay</sup><sup>az</sup><sup>ba</sup><sup>bb</sup><sup>bc</sup><sup>bd</sup><sup>be</sup><sup>bf</sup><sup>bg</sup><sup>bh</sup><sup>bi</sup><sup>bj</sup><sup>bk</sup><sup>bl</sup><sup>bm</sup><sup>bn</sup><sup>bo</sup><sup>bp</sup><sup>bq</sup><sup>br</sup><sup>bs</sup><sup>bt</sup><sup>bu</sup><sup>bv</sup><sup>bw</sup><sup>bx</sup><sup>by</sup><sup>bz</sup><sup>ca</sup><sup>cb</sup><sup>cc</sup><sup>cd</sup><sup>ce</sup><sup>cf</sup><sup>cg</sup><sup>ch</sup><sup>ci</sup><sup>cj</sup><sup>ck</sup><sup>cl</sup><sup>cm</sup><sup>cn</sup><sup>co</sup><sup>cp</sup><sup>cq</sup><sup>cr</sup><sup>cs</sup><sup>ct</sup><sup>cu</sup><sup>cv</sup><sup>cw</sup><sup>cx</sup><sup>cy</sup><sup>cz</sup><sup>ca</sup><sup>cb</sup><sup>cc</sup><sup>cd</sup><sup>ce</sup><sup>cf</sup><sup>cg</sup><sup>ch</sup><sup>ci</sup><sup>cj</sup><sup>ck</sup><sup>cl</sup><sup>cm</sup><sup>cn</sup><sup>co</sup><sup>cp</sup><sup>cq</sup><sup>cr</sup><sup>cs</sup><sup>ct</sup><sup>cu</sup><sup>cv</sup><sup>cw</sup><sup>cx</sup><sup>cy</sup><sup>cz</sup><sup>ca</sup><sup>cb</sup><sup>cc</sup><sup>cd</sup><sup>ce</sup><sup>cf</sup><sup>cg</sup><sup>ch</sup><sup>ci</sup><sup>cj</sup><sup>ck</sup><sup>cl</sup><sup>cm</sup><sup>cn</sup><sup>co</sup><sup>cp</sup><sup>cq</sup><sup>cr</sup><sup>cs</sup><sup>ct</sup><sup>cu</sup><sup>cv</sup><sup>cw</sup><sup>cx</sup><sup>cy</sup><sup>cz</sup><sup>ca</sup><sup>cb</sup><sup>cc</sup><sup>cd</sup><sup>ce</sup><sup>cf</sup><sup>cg</sup><sup>ch</sup><sup>ci</sup><sup>cj</sup><sup>ck</sup><sup>cl</sup><sup>cm</sup><sup>cn</sup><sup>co</sup><sup>cp</sup><sup>cq</sup><sup>cr</sup><sup>cs</sup><sup>ct</sup><sup>cu</sup><sup>cv</sup><sup>cw</sup><sup>cx</sup><sup>cy</sup><sup>cz</sup><sup>ca</sup><sup>cb</sup><sup>cc</sup><sup>cd</sup><sup>ce</sup><sup>cf</sup><sup>cg</sup><sup>ch</sup><sup>ci</sup><sup>cj</sup><sup>ck</sup><sup>cl</sup><sup>cm</sup>

<sup>a</sup> X<sup>c</sup>, Y<sup>c</sup> and Z<sup>c</sup> are the fractional coordinates of the centroid of the rigid group.

<sup>b</sup> The rigid group orientation angles Delta, Epsilon and Eta (radians) are the angles by which the rigid body is rotated with respect to a set of axes X, Y and Z. The origin is the centre of the ring; X is parallel to a\*, Z is parallel to c and Y is parallel to the line defined by the intersection of the plane containing a\* and b\* with the plane containing b and c.

TABLE 6. Idealized Positional and Thermal Parameters For the Hydrogen Atoms of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$ .

Atom	X	Y	Z	B(A <sup>2</sup> )	Atom	X	Y	Z	B(A <sup>2</sup> )
H(1C3)	0.2662	0.2099	0.4060	3.70	H(45)	-0.1094	0.2562	0.4534	6.03
H(2C3)	0.3434	0.1462	0.3411	3.70	H(46)	0.0370	0.1634	0.4098	5.02
H(1C4)	0.4592	0.0936	-0.0895	4.04	H(52)	0.2953	0.3953	-0.0238	4.72
H(2C4)	0.4253	0.1405	-0.1884	4.04	H(53)	0.2274	0.5034	-0.1313	5.71
H(12)	0.4893	0.4308	0.3517	6.07	H(54)	0.2871	0.5042	-0.3011	5.83
H(13)	0.6308	0.4565	0.4678	7.09	H(55)	0.4145	0.3970	-0.3634	5.88
H(14)	0.6840	0.3508	0.5842	6.22	H(56)	0.4824	0.2889	-0.2559	5.08
H(15)	0.5955	0.2193	0.5846	5.75	H(62)	0.5944	0.3827	-0.0213	6.05
H(16)	0.4540	0.1936	0.4685	4.97	H(63)	0.7691	0.3917	-0.0512	6.79
H(22)	0.2545	0.3578	0.4887	4.97	H(64)	0.8664	0.2632	-0.1184	7.32
H(23)	0.1345	0.4757	0.5395	5.86	H(65)	0.7890	0.1257	-0.1558	8.52
H(24)	0.0712	0.5738	0.4180	6.34	H(66)	0.6144	0.1166	-0.1258	6.53
H(25)	0.1281	0.5541	0.2456	6.44	H(72)	0.3994	-0.0084	-0.2493	5.92
H(26)	0.2482	0.4362	0.1947	5.42	H(73)	0.3970	-0.1621	-0.3075	7.40
H(32)	0.0308	0.0352	0.1970	5.72	H(74)	0.2779	-0.2505	-0.2417	7.47
H(33)	-0.0193	0.0978	0.2558	6.52	H(75)	0.1613	-0.1851	-0.1176	7.87
H(34)	0.0781	-0.1635	0.3887	7.65	H(76)	0.1638	-0.0314	-0.0594	6.34
H(35)	0.2255	-0.0962	0.4628	7.53	H(82)	0.2636	0.0918	-0.3257	5.54
H(36)	0.2756	0.0368	0.4040	5.62	H(83)	0.1769	0.1720	-0.4536	6.50
H(42)	0.0824	0.3085	0.1676	5.19	H(84)	0.0729	0.3013	-0.4027	6.52
H(43)	-0.0640	0.4013	0.2112	6.24	H(85)	0.0556	0.3504	-0.2240	6.16
H(44)	-0.1600	0.3751	0.3541	6.39	H(86)	0.1424	0.2702	-0.0962	5.09

Table 7. Least-Squares Plane Calculations

Plane no.	Equation <sup>a</sup>
1	-0.9474X+0.0789Y-0.3102Z+5.4077 = 0.0
2	-0.2057X-0.9781Y-0.0322Z+2.5719 = 0.0
3	-0.5894X+0.7959Y-0.2052Z+0.3962 = 0.0
4	-0.5653X+0.7961Y-0.2152Z+0.3913 = 0.0
5	0.2996Z-0.0306Y-0.9536Z+0.0220 = 0.0

## Deviations from the Planes (Å)

Atom	Plane no.				
	1	2	3	4	5
Rh(1)	-0.0093(5)				
Rh(2)					
Cl					
P(1)	-0.0092(14)	-0.0077(5)	-0.0058(5)	-0.0043(5)	-0.0002(4)
P(2)	0.0688(16)	0.0042(14)	0.0057(5)	0.0042(5)	-0.0001(4)
P(3)			0.0695(15)		0.0012(14)
P(4)	0.0684(15)	0.0384(16)	-0.0691(15)		
O(1)		0.0393(16)		0.0519(16)	0.056(6) <sup>b</sup>
O(2)	-0.522(7) <sup>b</sup>	0.417(8) <sup>b</sup>		-0.0517(16)	0.031(6) <sup>b</sup>
C(1)					0.031(6)
C(2)	-0.293(7)	0.214(8)			0.014(6)
C(3)			-0.708(6) <sup>b</sup>		
C(4)				-0.678(6) <sup>b</sup>	

## Dihedral Angle Between Planes

Plane A	Plane B	Angle(deg)
1	2	82.66
3	5	89.95
4	5	89.31

<sup>a</sup>X, Y, and Z are the orthogonal coordinates (Å) with X along the a axis, Y in the (a-b) plane and Z along C\*-axis.

<sup>b</sup>Not included in least squares plane calculation.

Table 8: Selected Distances (Å) in  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$ 

## Bond Distances

Rh(1)-Cl	2.406(2)		P(1)-C(11)	1.832(4)	} 1.822(5)	
Rh(2)-Cl	2.380(2)		P(1)-C(21)	1.825(3)		
Rh(1)-C(1)	1.807(7)		P(2)-C(31)	1.821(4)		
Rh(2)-C(2)	1.799(7)		P(2)-C(41)	1.823(3)		
Rh(1)-P(1)	2.324(2)	} 2.321(2) <sup>a</sup>	P(3)-C(51)	1.819(3)		
Rh(1)-P(3)	2.320(2)		P(3)-C(61)	1.819(4)		
Rh(2)-P(2)	2.319(2)		P(4)-C(71)	1.818(4)		
Rh(2)-P(4)	2.322(2)		P(4)-C(81)	1.822(4)		
C(1)-O(1)	1.184(8)		B(1)-F(1)	1.49(1)		} 1.38(10)
C(2)-O(2)	1.202(9)		B(1)-F(2)	1.39(1)		
P(1)-C(3)	1.825(6)	B(1)-F(3)	1.39(2)			
P(2)-C(3)	1.843(6)	B(1)-F(4)	1.47(4)			
P(3)-C(4)	1.841(6)	B(2)-F(5)	1.33(2)			
P(4)-C(4)	1.836(6)	B(2)-F(6)	1.51(1)			
		B(2)-F(7)	1.25(3)			
		B(2)-F(8)	1.24(3)			

## Nonbonded Distances

Rh(1)-Rh(2)	3.1520(8)	Cl-H1C4	2.90
P(1)-P(2)	3.088(2)	C(1)-H(52)	2.63
P(3)-P(4)	3.097(2)	C(2)-H(86)	2.72
O(1)-H(26)	2.86	F(1)-H(16)	2.37
O(1)-H(12)	2.87	F(1)-H(2)	2.37
O(1)-H(62)	2.89	F(3)-H(16)	2.35
O(2)-H(75)	2.76	F(3)-H(36)	2.38
C(1)-H(26)	2.61	H(36)-H(2)	2.15
Cl-H2C3	2.85	H(66)-H(3)	2.15

<sup>a</sup>For averaged quantities, the estimated standard deviation is the larger of an individual standard deviation or the standard deviation of a single observation as calculated from the mean.

Table 9: Selected Angles (Deg) in  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BF}_4]$ 

Bond Angles			
Cl-Rh(1)-C(1)	170.9(2)	C(11)-P(1)-C(21)	102.2(2)
Cl-Rh(1)-P(1)	90.44(5)	C(31)-P(2)-C(41)	102.4(2)
Cl-Rh(1)-P(3)	89.68(5)	C(51)-P(3)-C(61)	102.6(2)
C(1)-Rh(1)-P(1)	91.0(2)	C(71)-P(4)-C(81)	105.8(2)
C(1)-Rh(1)-P(3)	89.5(2)	P(1)-C(3)-P(2)	114.7(3)
P(1)-Rh(1)-P(3)	176.20(6)	P(3)-C(4)-P(4)	114.7(3)
Cl-Rh(2)-C(2)	172.6(3)	P(1)-C(11)-C(12)	117.0(3)
Cl-Rh(2)-P(2)	88.59(5)	P(1)-C(11)-C(16)	122.8(3)
Cl-Rh(2)-P(4)	88.28(5)	P(1)-C(21)-C(22)	118.5(2)
C(2)-Rh(2)-P(2)	91.7(2)	P(1)-C(21)-C(26)	121.5(2)
C(2)-Rh(2)-P(4)	91.1(2)	P(2)-C(31)-C(32)	116.5(3)
P(2)-Rh(2)-P(4)	176.12(6)	P(2)-C(31)-C(36)	123.4(3)
Rh(1)-Cl-Rh(2)	82.38(5)	P(2)-C(41)-C(42)	119.4(2)
Rh(1)-C(1)-O(1)	177.4(7)	P(2)-C(41)-C(46)	120.6(2)
Rh(2)-C(2)-O(2)	177.0(8)	P(3)-C(51)-C(52)	121.0(2)
Rh(1)-P(1)-C(3)	112.6(2)	P(3)-C(51)-C(56)	119.0(2)
Rh(2)-P(2)-C(3)	112.8(2)	P(3)-C(61)-C(62)	116.9(3)
Rh(1)-P(3)-C(4)	113.6(2)	P(3)-C(61)-C(66)	123.0(3)
Rh(2)-P(4)-C(4)	113.8(2)	P(4)-C(71)-C(72)	121.9(3)
Rh(1)-P(1)-C(11)	113.9(2)	P(4)-C(71)-C(76)	118.1(3)
Rh(1)-P(1)-C(21)	118.7(1)	P(4)-C(81)-C(82)	120.1(3)
Rh(2)-P(2)-C(31)	112.6(2)	P(4)-C(86)-C(86)	119.9(3)
Rh(2)-P(2)-C(41)	117.8(1)	F(1)-B(1)-F(2)	103.5(7)
Rh(1)-P(3)-C(51)	115.9(1)	F(1)-B(1)-F(3)	102.8(9)
Rh(1)-P(3)-C(61)	115.5(2)	F(1)-B(1)-F(4)	111(1)
Rh(2)-P(4)-C(71)	111.5(2)	F(2)-B(1)-F(3)	111.6(9)
Rh(2)-P(4)-C(81)	118.8(2)	F(2)-B(1)-F(4)	105(1)
C(3)-P(1)-C(11)	103.9(2)	F(3)-B(1)-F(4)	122(1)
C(3)-P(1)-C(21)	103.8(2)	F(5)-B(2)-F(6)	93(2)
C(3)-P(2)-C(31)	103.5(2)	F(5)-B(2)-F(7)	110(1)
C(3)-P(2)-C(41)	106.2(2)	F(5)-B(2)-F(8)	122(2)
C(4)-P(3)-C(51)	104.5(2)	F(6)-B(2)-F(7)	99(2)
C(4)-P(3)-C(61)	103.0(2)	F(6)-B(2)-F(8)	106(2)
C(4)-P(4)-C(71)	102.5(3)	F(7)-B(2)-F(8)	120(2)
C(4)-P(4)-C(81)	102.8(2)		

Torsion Angles			
P(1)-Rh(1)-Rh(2)-P(2)	3.70(5)	C(2)-Rh(2)-P(4)-C(71)	85.3(3)
P(1)-Rh(1)-Rh(2)-P(4)	179.84(6)	C(2)-Rh(2)-P(4)-C(81)	-38.1(3)
P(2)-Rh(2)-Rh(1)-P(3)	-178.90(6)	C(11)-P(1)-P(2)-C(31)	8.5(3)
P(3)-Rh(1)-Rh(2)-P(4)	-2.76(6)	C(11)-P(1)-P(3)-C(61)	-1.4(2)
C(1)-Rh(1)-P(1)-C(11)	72.9(3)	C(21)-P(1)-P(2)-C(41)	3.0(2)
C(1)-Rh(1)-P(1)-C(21)	-47.6(3)	C(21)-P(1)-P(3)-C(51)	-1.8(2)
C(1)-Rh(1)-P(3)-C(51)	45.9(3)	C(31)-P(2)-P(4)-C(71)	1.2(2)
C(1)-Rh(1)-P(3)-C(61)	-74.2(3)	C(41)-P(2)-P(4)-C(81)	-3.4(3)
C(2)-Rh(2)-P(2)-C(31)	-84.0(3)	C(51)-P(3)-P(4)-C(81)	-5.6(2)
C(2)-Rh(2)-P(2)-C(41)	34.9(3)	C(61)-P(3)-P(4)-C(71)	-11.3(4)



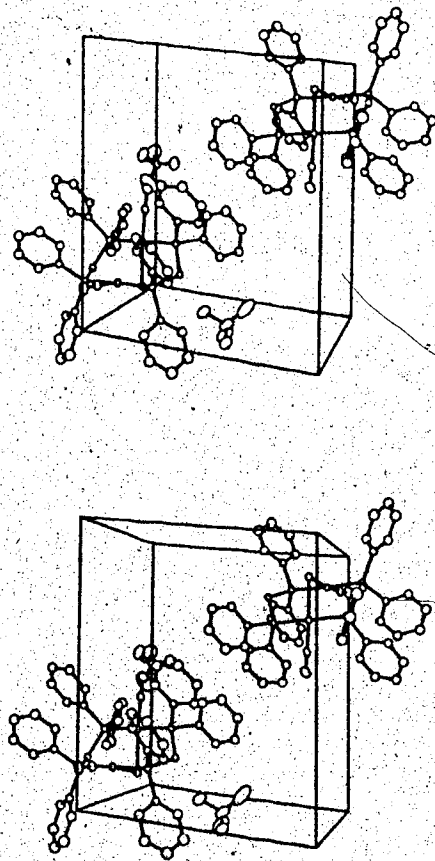


Figure 4. Cell Packing Diagram of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^-$

$[\text{BF}_4]$ .

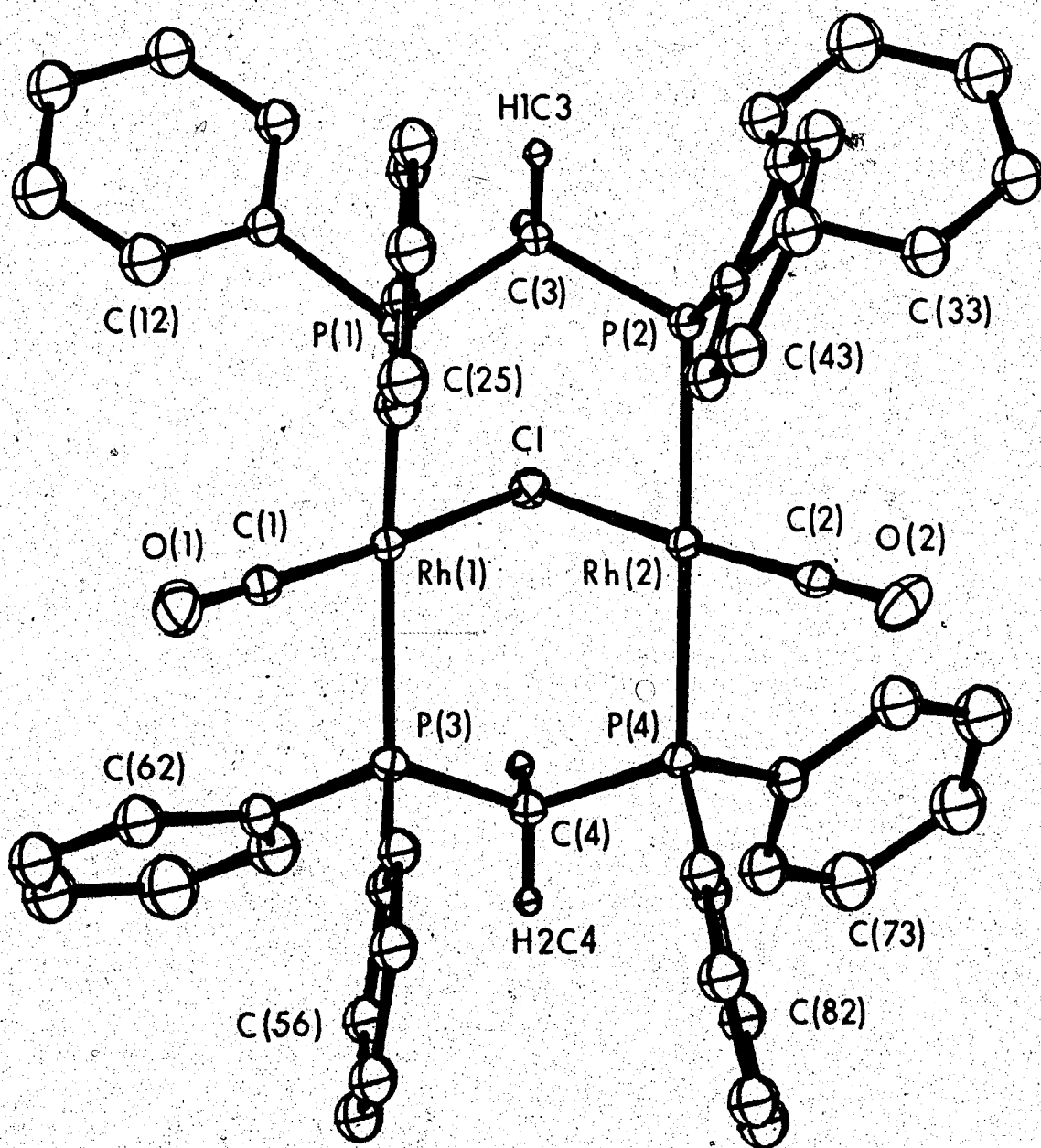


Figure 5. A Perspective View of the  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  Cation.

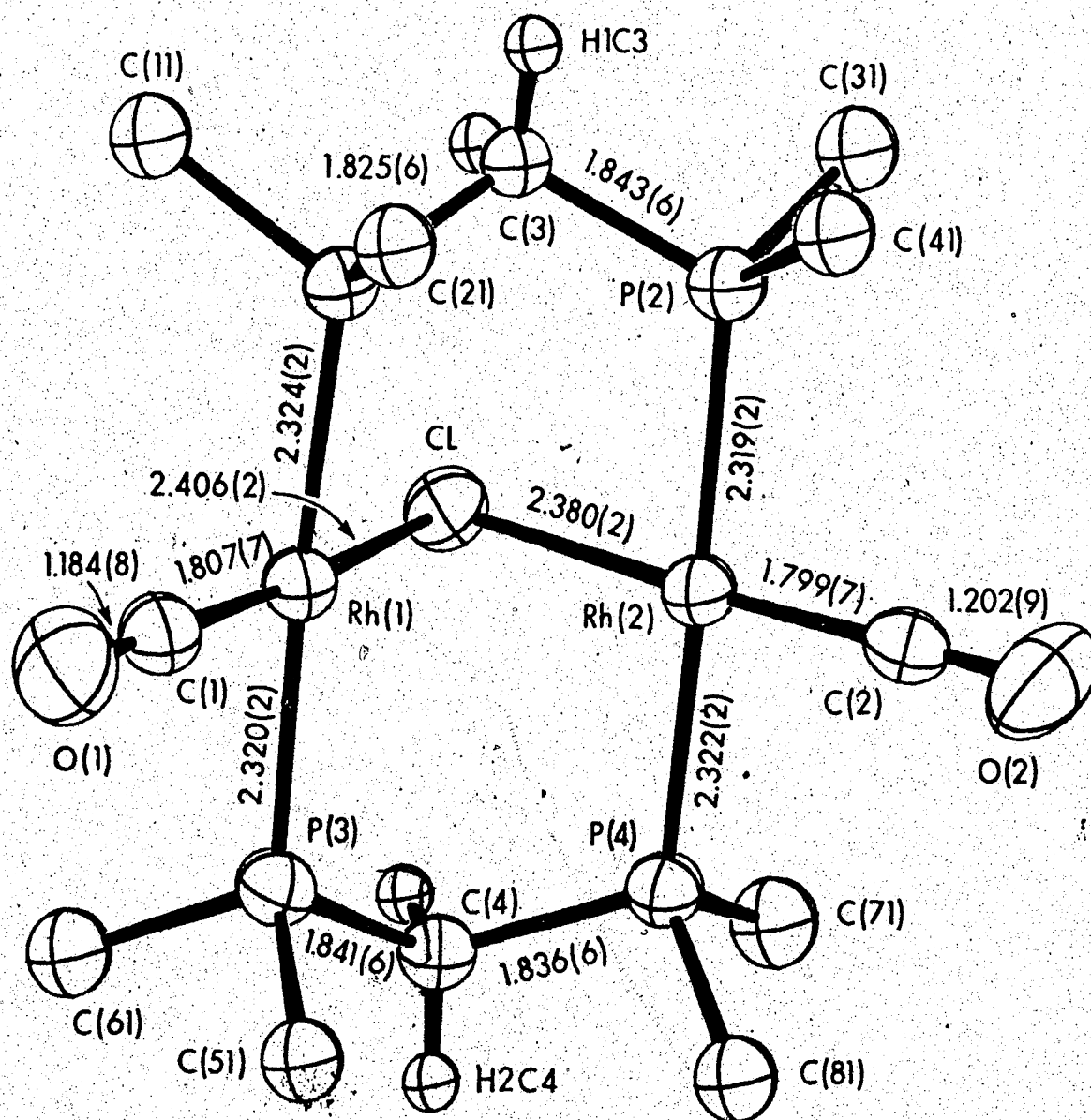


Figure 6. The Inner Coordination Sphere of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  Cation.

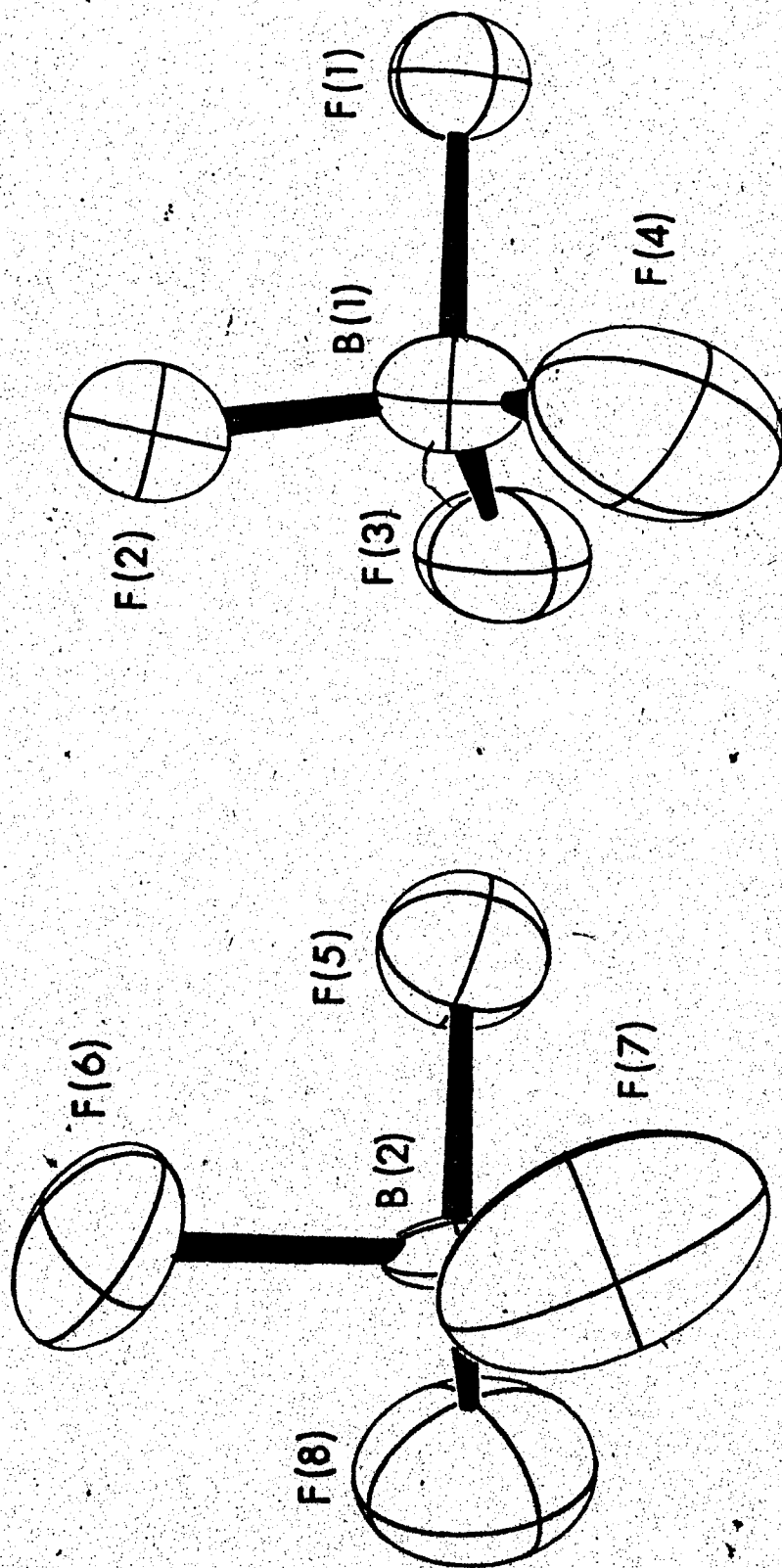


Figure 7. The Two Independent Tetrafluoroborate Anions.

DESCRIPTION OF STRUCTURE

The two independent  $\text{BF}_4^-$  anions, although inversion disordered and undergoing a large amount of thermal vibration, show reasonable tetrahedral geometries (see Figure 4). The range in the B-F distances (1.24(3)-1.51(1) Å) and the F-B-F angles (93(2)-122(2)°) are not unreasonable considering the observed disorder and thermal motion, suggesting that the refined model is acceptable. These values are in reasonable agreement with other structural determinations involving  $\text{BF}_4^-$  salts.<sup>111</sup> The only significant nonbonded contacts involving the  $\text{BF}_4^-$  anion are between the fluorine atoms and the phenyl hydrogen atoms (see Table 8). These distances (2.35-2.38 Å) are somewhat shorter than the sum of their van der Waal's radii (2.57)<sup>112</sup> and may explain the orientations of the phenyl rings and the relatively open bridging site, between the two rhodium centres (vide infra).

The  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  cation displays the expected "A-frame" geometry in which the rhodium atoms are bridged by two DPM ligands which are mutually trans. The chloro ligand bridges the two metal centres in the equatorial plane perpendicular to the Rh-P vectors, and the carbonyl ligands, also lying in this plane, are bonded to each Rh atom trans to the bridging Cl atom. Both Rh atoms display slightly distorted square-planar geometries, whose least-square planes are inclined to each other by 82.66°.

The distortions from square planar geometry seem to result from close nonbonded contacts between the carbonyl ligands and the hydrogen atoms of the endo phenyl groups which enclose the bridging site. Indeed the larger distortion, about Rh(1), is accompanied by the shortest nonbonded contacts, involving C(1) and O(1) (see Table 8).

The relatively long Rh...Rh separation of  $3.1520(8)\text{\AA}$  is consistent with no formal Rh-Rh bond. This distance is significantly longer than the Rh-Rh distance of  $2.8415(7)\text{\AA}$  observed in the carbonyl adduct  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2]\text{-}[\text{BPh}_4]$  (2),<sup>35</sup> where all evidence suggests the presence of a formal Rh-Rh single bond. The absence of a formal Rh-Rh bond in the present complex is substantiated by the following structural parameters: i) the Rh-Rh separation is significantly greater than the intraligand P...P separations of  $3.088(2)$  and  $3.097(2)\text{\AA}$ , (when the metals are mutually bonded the converse is true);<sup>35b</sup> ii) the Rh(1)-Cl-Rh(2) angle of  $82.38(5)^\circ$  compares well with values typically observed when no formal metal-metal bond is present (range  $80\text{-}95^\circ$ )<sup>113-116</sup> and contrasts to the value of  $66.51(4)^\circ$  observed in the Rh-Rh bonded carbonyl adduct 2. In addition, the absence of a formal metal-metal bond is required to explain the observed diamagnetism and to give each rhodium atom a 16-electron configuration.

The Rh-Cl distances of  $2.406(2)$  and  $2.380(2)\text{\AA}$  are in the range typically observed in other chloro-bridged dimer

systems (ca. 2.30-2.45 Å)<sup>113-116</sup> and are significantly shorter than those observed in the carbonyl adduct 2 (2.575(2) and 2.607(2) Å).<sup>35</sup> The observed asymmetry in these parameters involving the chloro ligand presumably results as a consequence of nonbonded contacts, since there is no *a priori* reason to expect a chemical difference in the two rhodium centres. In support of this argument, the shortest nonbonded contacts involving the chloro ligands are H2C3-Cl and H1C4-Cl (2.80-2.90 Å, respectively). These interactions act in such a way as to force the bridging chloro ligand out of the symmetrical position towards Rh(2). This chloride asymmetry is reflected in the parameters of the carbonyl groups which are trans to the Cl atom. Although not statistically significant, the trend in the carbonyl parameters is consistent with the chloro ligand acting as a weaker  $\pi$ -donor to Rh(1) than to Rh(2) with the concomitant result that C(1)O(1) has a weaker  $\pi$ -accepting ability compared to C(2)O(2) (Rh(1)-C(1) = 1.807(7) Å, C(1)-O(1) = 1.184(8) Å, Rh(2)-C(2) = 1.799(7) Å, C(2)-O(2) = 1.202(9) Å). No other short contacts are observed that would readily explain the observed asymmetry in the chloro ligand. The slight bend in both carbonyl ligands (Rh-C-O(av) = 177.2(8)°) is not unusual and is probably also steric in origin.

Within the Rh-DPM framework the parameters are not unusual. The Rh-P distances (average 2.321(2) Å) compare well with other Rh-DPM<sup>35,88-90,96</sup> systems and are typical for Rh(1)-phosphine distances when trans to another phos-

phine ligand (e.g., 2.322(4) and 2.338(4) Å in red and orange Wilkinson's catalyst).<sup>117</sup> The P-C distances (both methylene and phenyl) are quite ordinary and the P-C-P angles (average 114.7(3)°) are close to the expected tetrahedral value as is typical when the DPM ligand bridges two metals.

The methylene groups of the DPM ligands are folded in a cis configuration, with both groups inclined towards the bridging chloro ligand. Therefore, C(3) is 0.708(6) Å out of the Rh(1)-P(1)-P(2)-Rh(2) plane and C(4) is 0.678(6) Å out of the Rh(1)-P(3)-P(4)-Rh(2) plane. This cis methylene orientation is quite typical of most analogous DPM and DAM bridged species.<sup>32,35,41,81,85,89</sup> In general the methylene groups bend towards the more sterically encumbered site; so for example when two bridging equatorial ligands are present, the folding is towards the more bulky of these bridging ligands. By folding in this manner the non-bonded contacts between the more bulky phenyl groups and the equatorial ligands are minimized. Further, in the present structure the cis methylene configuration results in a phenyl ring orientation which allows relatively free access to the bridging site, between the Rh atoms and opposite the chloro ligand. The trans configuration of the methylene groups has been observed<sup>31,32,83b,118</sup> when there is no steric preference for one side of the Rh-phosphine framework over the other.



Viewed along the Rh-Rh axis the Rh-P vectors on adjacent rhodium atoms are close to eclipsed as is evidenced by the small P-Rh(1)-Rh(2)-P torsion angles ( $0.16(6)$  to  $3.70(5)^\circ$ , see Table 9). This presents an interesting contrast to that observed in the analogous sulfido bridged species,  $[\text{Rh}_2(\text{CO})_2^-(\mu\text{-S})(\text{DPM})_2]^{89}$  (3), which appears to be severely twisted about the Rh-Rh axis. Model building has shown that this twist about the Rh-Rh axis in "A-frame" complexes results in two of the endo phenyl rings moving into the bridging site, thereby effectively blocking this site, as was observed in the sulfido bridged species. The orientation of the phenyl rings in the present species, however is such that the bridging site is more accessible than in the sulfido complex. It is difficult, however, in the present case to draw analogies between the solution chemistries and the solid state structures since the observed differences in phosphine twists between 1 and 3 may be a result of crystal packing. Indeed in the present complex the  $\text{BF}_4^-$  anion at the 1(c) inversion centre sits directly above the bridging site (see Figure 4) and displays non-bonded contacts with the hydrogen atoms of the surrounding phenyl rings which are shorter than van der Waal's distances<sup>112</sup> (vide supra). It is expected that the  $\text{BF}_4^-$  anion, in this position, exerts considerable influence on the orientations of these phenyl groups and hence on the crowding of the bridging site. Certainly there is no obvious chemical reason to explain the twist difference in the two otherwise similar compounds.

## DISCUSSION

The crystallization of 1 as the  $\text{BF}_4^-$  salt was somewhat of a surprise, considering that the anions initially present were  $\text{PF}_6^-$  and  $\text{BPh}_4^-$ . There are two obvious sources of this  $\text{BF}_4^-$  anion. The first is through fluorination of  $\text{BPh}_4^-$  anion by HF, which is known to be present in acetone solutions of  $\text{PF}_6^-$ , and the second is through leaching of boron from the borosilicate glass by HF. On the basis of  $^{31}\text{P}$  and  $^{19}\text{F}$  NMR studies, it seems that the latter is more likely. When complex 1 and  $[\text{N}_2\text{Ph}][\text{PF}_6]$  are reacted in acetone and the mixture left for several weeks the NMR spectra indicated that the  $\text{PF}_6^-$  concentration is greatly diminished, and shows the presence of fluorosilanes,  $\text{BF}_4^-$  and other unidentified species. Furthermore, the NMR tubes and glassware used in the crystallizations were found to be etched, suggesting that significant leaching of the glass had occurred. In any case the well formed crystals were a pleasant surprise since all known previous attempts to obtain suitable single crystals of complex 1 with other anions had failed.<sup>119</sup>

Although the present structure seems significantly different than that of the sulfido bridged analogue 3 with respect to crowding of the bridging site, it is believed that this is a consequence more of solid-state effects than of chemical differences. Any differences in the chemistries of these two species that might occur are more likely a conse-

quence of the difference in bridging ligands ( $S^{2-}$  and  $Cl^-$ ) and the overall charge of the species. In this regard it will be of obvious interest to compare the chemistries of these species.

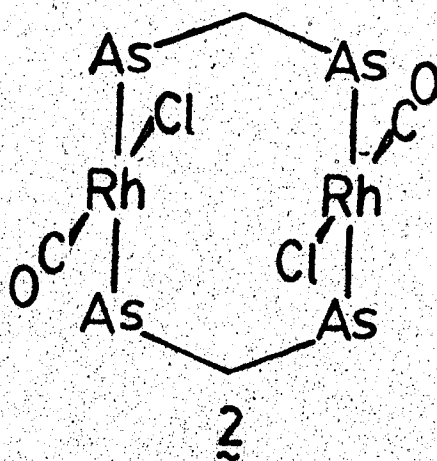
The present structure verifies that the bridging site in DPM-bridged species is accessible to small molecules and therefore it is not unexpected that some small molecules, such as  $SO_2$ , are capable of attack at this site, as the experimental evidence suggests (Chapter IV). It is however, not obvious, based on this structure determination, why some small molecules attack at the bridging site and others attack at the terminal site,

## CHAPTER III.

### The Structure of *trans*-[RhCl(CO)(DPM)]<sub>2</sub>

#### INTRODUCTION

The reactions of *trans*-[RhCl(CO)(DPM)]<sub>2</sub> (1) with small molecules were investigated as part of our studies into the chemistry of DPM-bridged binuclear rhodium complexes.<sup>35,96</sup> Although the structure of compound 1 had not been determined, it was believed, on the basis of X-ray powder diffraction studies,<sup>66</sup> to be the same as the DAM-bridged analogue, *trans*-[RhCl(CO)(DAM)]<sub>2</sub> (2),<sup>31</sup> whose structure is known and whose framework is sketched below:



Unlike the "A-frame" species (see Chapter II),<sup>120</sup> only the terminal sites above the square planar metal atoms in 1 and 2 are open to attack since the sites between the metals are blocked by the chloro and carbonyl ligands.

In spite of the proposed structural analogies in compounds 1 and 2,<sup>66</sup> however, significant differences in their chemistries led us to question the extent of their similarities. It had been noted, for example, that "ketonic" carbonyl complexes of Pt and Pd were more stable with DAM than with DPM,<sup>32,41,84</sup> whereas our work tended to indicate that the opposite was true with rhodium. In species containing unsupported bridging ligands, such as the "ketonic" carbonyl ligand, we anticipated that the metal-metal separation might be an important factor in determining the stability of the unsupported ligand complex. Since the obvious difference in the DPM and DAM ligands lies in their ligand bites, due to the greater size of As compared to P, and since the DAM ligand would therefore tend to prefer larger metal-metal separations than DPM, it was deemed important to obtain structural information on the DPM complex 1 in order to compare the metal-metal separations and the subsequent effects on ligand orientations in the two compounds 1 and 2.

Furthermore, we prepared an isomer of 1,<sup>96</sup> which appears to be the cis-dichlorodicarbonyl species (see Chapter IV). This isomer has a greatly differing solubility and chemistry with CO compared to the trans isomer 1 so structural comparisons of the two species seemed in order. Therefore, when reaction of 1 (of which suitable, single crystals had never been obtained by us) with CS<sub>2</sub> resulted in the serendipitous crystallization of well formed rhombs of complex 1, it was decided to undertake its structural

determination.

### EXPERIMENTAL

#### Crystallization of *trans*-[RhCl(CO)(DPM)]<sub>2</sub>

To a suspension of 0.100 g (0.091 mmol) of *trans*-[RhCl(CO)(DPM)]<sub>2</sub><sup>66</sup> in 15 mL of CH<sub>2</sub>Cl<sub>2</sub> was added 15 mL of CS<sub>2</sub>. After one hour diethyl ether was added to the clear red solution to induce crystallization. The red solid obtained was then redissolved in 15 mL of CH<sub>2</sub>Cl<sub>2</sub> from which well formed yellow crystals were obtained by diethyl ether diffusion. Chemical and spectral analysis showed that the crystals were the starting material, complex 1.

#### Data Collection

A clear yellow plate of *trans*-[RhCl(CO)(DPM)]<sub>2</sub> was mounted on a glass fiber. Preliminary film data showed  $\bar{1}$  Laue symmetry and no systematic absences, consistent with the space groups P1 or  $\bar{P}1$ . The centrosymmetric space group was chosen and later verified by the successful refinement of the structure with acceptable positional parameters, thermal parameters and agreement indices and the location of all hydrogen atoms in the electron density difference maps. A cell reduction<sup>102</sup> failed to show the presence of higher symmetry. The reduced cell is reported and is presented together with the pertinent crystal data and details of data collection are in Table 10. Otherwise data collection proceeded as described in Chapter II.

Table 10. Summary of Crystal Data and Intensity Collection  
for *trans*-[RhCl(CO)(DPM)]<sub>2</sub>

Compound	<i>trans</i> -[RhCl(CO)(DPM)] <sub>2</sub>																												
Formula	C <sub>52</sub> H <sub>44</sub> Cl <sub>2</sub> O <sub>2</sub> P <sub>4</sub> Rh <sub>2</sub>																												
Formula Weight	1101.54 amu																												
Reduced Cell Parameters																													
a	11.0542(11) Å																												
b	12.5640(10) Å																												
c	10.3191(9) Å																												
γ	99.899(6)°																												
β	115.708(7)°																												
α	65.082(7)°																												
V	1171.0 Å <sup>3</sup>																												
Z	1																												
Density	1.562 g·cm <sup>-3</sup> (calc'd.) 1.565(5) g·cm <sup>-3</sup> (expt'l. by flotation)																												
Space Group	C <sub>i</sub> <sup>1</sup> - P $\bar{1}$																												
Crystal Dimensions	0.346 x 0.555 x 0.077 mm																												
Crystal Volume	0.0094 mm <sup>3</sup>																												
Crystal Faces (and distances from an arbitrary origin within the crystal (mm))	<table border="0"> <tbody> <tr> <td>1</td> <td>1</td> <td>0</td> <td>(0.114)</td> </tr> <tr> <td><math>\bar{1}</math></td> <td><math>\bar{1}</math></td> <td>0</td> <td>(0.114)</td> </tr> <tr> <td>0</td> <td>1</td> <td>0</td> <td>(0.035)</td> </tr> <tr> <td>0</td> <td><math>\bar{1}</math></td> <td>0</td> <td>(0.035)</td> </tr> <tr> <td>0</td> <td>0</td> <td>1</td> <td>(0.250)</td> </tr> <tr> <td>0</td> <td>0</td> <td><math>\bar{1}</math></td> <td>(0.250)</td> </tr> <tr> <td>0</td> <td><math>\bar{1}</math></td> <td><math>\bar{1}</math></td> <td>(0.192)</td> </tr> </tbody> </table>	1	1	0	(0.114)	$\bar{1}$	$\bar{1}$	0	(0.114)	0	1	0	(0.035)	0	$\bar{1}$	0	(0.035)	0	0	1	(0.250)	0	0	$\bar{1}$	(0.250)	0	$\bar{1}$	$\bar{1}$	(0.192)
1	1	0	(0.114)																										
$\bar{1}$	$\bar{1}$	0	(0.114)																										
0	1	0	(0.035)																										
0	$\bar{1}$	0	(0.035)																										
0	0	1	(0.250)																										
0	0	$\bar{1}$	(0.250)																										
0	$\bar{1}$	$\bar{1}$	(0.192)																										
Temperature	20°C																												
Radiation	CuKα (λ=1.540562 Å) filtered with 0.5 mil thick nickel foil																												
μ	85.439 cm <sup>-1</sup>																												
Range in Absorption Correction Factors	0.140 - 0.567																												
Receiving Aperture	4x4 mm, 30 cm from the crystal																												

Table 10, continued

Takeoff Angle	4.1°
Scan Speed	2° in 2θ/min
Scan Range	1.00 below $K_{\alpha 1}$ to 1.00 above $K_{\alpha 2}$
Background Counting Time	10s ( $3^\circ < 2\theta < 60^\circ$ ) 20s ( $60^\circ < 2\theta < 120^\circ$ )
2θ limits	$3.0^\circ < 2\theta < 120.0^\circ$
2θ limits for centered reflections	$60^\circ < 2\theta < 70^\circ$
Final number of variables	113
Unique Data Collected	3505
Unique Data Used ( $F_o^2 \geq 3\sigma(F_o^2)$ )	3368
Error in observation of unit weight	1.866
R	0.037
$R_w$	0.069



### Solution of Structure

The independent Rh atom position was obtained from a sharpened Patterson map. Subsequent least-squares calculations and electron density difference maps led to the location of all other atoms. Anomalous dispersion terms<sup>108</sup> for Rh, P and Cl were included in  $F_C$ . The carbon atoms of the phenyl rings were refined as rigid groups. Hydrogen atoms were included as fixed contributions and not refined. All nongroup atoms were refined individually with anisotropic thermal parameters (for a more detailed discussion of structure solution and rigid group treatment see Chapter II).

The final model with 115 parameters varied converged to  $R=0.037$  and  $R_w=0.069$ .<sup>121</sup> In the final electron density difference map all of the highest 20 peaks were in the vicinities of the phenyl rings ( $0.91-0.54 \text{ e}/\text{\AA}^3$ ). A typical carbon atom on an earlier electron density difference map had an electron density of  $7.7 \text{ e}/\text{\AA}^3$ .

### Results

The final positional and thermal parameters for the nongroup and group atoms are given in Tables 11 and 12, respectively. The idealized positional and thermal parameters for the hydrogen atoms are given in Table 13. Least squares plane calculations are presented in Table 14 and selected bond distances and angles are given in Tables 15 and 16, respectively. A listing of observed and calculated structure amplitudes is available.<sup>110</sup> The unit cell of

*trans*-[RhCl(CO)(DPM)]<sub>2</sub> is shown in Figure 8. Four adjacent molecules are drawn in order to show some of the packing interactions. The crystallographic *b* axis runs from bottom to top of the page, the *c* axis is horizontal to the right and the *a* axis runs into the page. Figure 9 presents a perspective view of the compound, including the numbering scheme (phenyl hydrogens have the same number as their attached carbon atom). The inner coordination sphere of *trans*-[RhCl(CO)(DPM)]<sub>2</sub> is shown in Figure 10, along with some relevant bond lengths, 50% thermal ellipsoids are drawn.

TABLE 11. Positional and Thermal Parameters For the Nongroup Atoms of Trans-[RhCl(CO)(DPM)]<sub>2</sub>.

Atom	<sup>a</sup> x	<sup>a</sup> y	<sup>a</sup> z	<sup>b</sup> U11	<sup>b</sup> U22	<sup>b</sup> U33	<sup>b</sup> U12	<sup>b</sup> U13	<sup>b</sup> U23
Rh	0.02710(2)	-0.04223(2)	0.15345(2)	2.36(2)	2.13(2)	2.83(2)	-0.68(1)	1.26(1)	0.09(1)
Cl	0.18334(8)	0.06132(8)	0.2207(1)	3.63(5)	3.77(5)	4.22(5)	-1.76(4)	1.70(4)	-0.16(4)
P(1)	-0.22241(9)	0.20635(7)	-0.13917(9)	2.63(5)	2.20(4)	3.00(5)	-0.64(3)	1.32(4)	0.24(3)
P(2)	-0.17744(9)	0.12221(7)	0.15280(9)	2.48(4)	2.34(4)	2.80(5)	-0.69(3)	1.32(4)	-0.01(3)
O(1)	-0.1297(4)	-0.1852(3)	0.1355(4)	7.1(2)	4.4(2)	10.3(3)	-2.9(2)	5.8(2)	-0.9(2)
C(1)	-0.0725(4)	-0.1309(3)	0.1376(5)	3.4(2)	3.4(2)	5.6(3)	-1.0(2)	2.4(2)	-1.2(2)
C(2)	-0.3019(3)	0.1755(3)	-0.0309(4)	2.6(2)	2.7(2)	2.9(2)	-0.7(1)	1.5(1)	-0.2(1)

<sup>a</sup> Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

<sup>b</sup> The form of the thermal ellipsoid is:  $\exp[-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a^2bU_{12}hk + 2a^2cU_{13}hl + 2b^2cU_{23}kl)]$ . The quantities given in the table are the thermal coefficients  $\times 10^3$ .

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TABLE 12. Derived Parameters for the Rigid Group Atoms of Trans-[RhCl(CO)(DPM)]<sub>2</sub>.

Atom	X	Y	Z	B(A <sup>2</sup> )	Atom	X	Y	Z	B(A <sup>2</sup> )
C(11)	-0.2018(3)	0.3442(2)	-0.0656(3)	2.48(6)	C(31)	-0.1562(3)	0.2475(2)	0.2675(3)	2.43(6)
C(12)	-0.3189(2)	0.4518(2)	-0.1109(2)	3.66(8)	C(32)	-0.0330(3)	0.2239(2)	0.3966(2)	3.61(8)
C(13)	-0.3039(2)	0.5548(2)	-0.0460(2)	4.71(9)	C(33)	-0.0182(4)	0.3131(3)	0.4952(2)	4.8(1)
C(14)	-0.1719(3)	0.5503(2)	0.0641(3)	4.9(1)	C(34)	-0.1265(3)	0.4259(2)	0.4648(3)	4.64(9)
C(15)	-0.0549(2)	0.4428(2)	0.1094(2)	4.34(9)	C(35)	-0.2496(3)	0.4495(2)	0.3351(2)	4.57(9)
C(16)	-0.0698(2)	0.3397(2)	0.0445(2)	3.09(7)	C(36)	-0.2645(4)	0.3603(3)	0.2371(2)	3.33(7)
C(21)	-0.3759(6)	0.2513(2)	-0.3143(2)	2.51(6)	C(41)	-0.2962(4)	0.0828(3)	0.2113(6)	2.25(6)
C(22)	-0.5019(5)	0.2311(3)	-0.3546(5)	3.10(7)	C(42)	-0.4395(5)	0.1074(2)	0.1225(4)	2.86(6)
C(23)	-0.6134(4)	0.2652(3)	-0.4909(3)	3.92(8)	C(43)	-0.5214(2)	0.0819(2)	0.1747(2)	3.29(7)
C(24)	-0.5989(6)	0.2194(2)	-0.5870(2)	4.30(8)	C(44)	-0.4600(4)	0.0420(3)	0.3157(6)	3.29(7)
C(25)	-0.4728(5)	0.3226(3)	-0.5469(5)	4.55(9)	C(45)	-0.3166(5)	0.0274(2)	0.4045(4)	3.83(8)
C(26)	-0.3614(4)	0.3055(3)	-0.4107(3)	3.67(8)	C(46)	-0.2347(2)	0.0529(2)	0.3524(2)	3.40(7)

## Rigid Group Parameters

	X <sub>c</sub>	Y <sub>c</sub>	Z <sub>c</sub>	Delta	Epsilon	Eta
Ring1	-0.1869(2)	0.4473(2)	-0.0007(2)	-0.231(2)	2.822(2)	4.892(1)
Ring2	-0.4874(2)	0.2854(2)	-0.4508(2)	0.916(2)	2.384(3)	3.127(3)
Ring3	-0.1413(2)	0.3367(2)	0.3662(2)	2.683(2)	2.597(2)	1.198(2)
Ring4	-0.3781(2)	0.0674(1)	0.2635(2)	4.237(2)	2.366(3)	4.823(3)

<sup>a</sup> X<sub>c</sub>, Y<sub>c</sub> and Z<sub>c</sub> are the fractional coordinates of the centroid of the rigid group.

<sup>b</sup> The rigid group orientation angles Delta, Epsilon and Eta (radians) are the angles by which the rigid body is rotated with respect to a set of axes X, Y and Z. The origin is the centre of the ring; X is parallel to a\*, Z is parallel to c and Y is parallel to the line defined by the intersection of the plane containing a\* and b\* with the plane containing b and c.

TABLE 13. Idealized Positional and Thermal Parameters For the Hydrogen Atoms of Trans-[RhCl(CO)(DPH)]<sub>2</sub>.

Atom	x	y	z	B(A <sup>2</sup> )	Atom	x	y	z	B(A <sup>2</sup> )
H(1)	-0.3433	0.1229	-0.0808	3.22	H(26)	-0.2751	0.3186	-0.3835	4.70
H(2)	-0.3770	0.2501	-0.0251	3.22	H(32)	0.0412	0.1466	0.4177	4.62
H(12)	-0.4080	0.4550	-0.1858	4.50	H(33)	0.0663	0.2969	0.5833	5.89
H(13)	-0.3839	0.6284	-0.0766	5.52	H(34)	-0.1158	0.4867	0.5319	5.64
H(14)	-0.1618	0.6209	0.1085	5.81	H(35)	-0.3232	0.5262	0.3150	5.49
H(15)	0.0359	0.4400	0.1845	5.39	H(36)	-0.3484	0.3759	0.1493	4.38
H(18)	0.0102	0.2666	0.0753	4.18	H(42)	-0.4814	0.1353	0.0266	3.85
H(22)	-0.5127	0.1947	-0.2891	3.89	C(43)	-0.6182	0.0921	0.1140	4.33
H(23)	-0.7000	0.2526	-0.5185	4.85	H(44)	-0.5159	0.0245	0.3511	4.40
H(24)	-0.6749	0.3426	-0.6803	5.18	H(45)	-0.2748	0.0001	0.5008	4.74
H(25)	-0.4625	0.3759	-0.6128	5.46	H(46)	-0.1370	0.0433	0.4134	4.31

Table 14. Least-Squares Plane Calculations

Plane no.	Equation
1	$-0.7174X - 0.5092Y - 0.4755Z + 0.0 = 0.0^a$
2	$0.1832X + 0.1661Y - 0.9689Z + 1.5689 = 0.0$

Deviations from the Planes (Å)

Plane no.	Atom			
	Rh	P(1)	P(2)	Cl
1	-0.0047(2)	-0.040(1)	0.040(1)	0.0608(9)
2	-0.0021(2)	0.0637(9)	0.0492(9)	-0.302(4)
			0	-0.553(4)
				0.720(4) <sup>b</sup>

Angle between Rh-Rh vector and plane 2 = 75.9°

<sup>a</sup>X, Y, and Z are orthogonal coordinates (Å) with X along the a axis, Y in the a-b plane and Z along the C<sup>∞</sup>-axis.

<sup>b</sup>Not included in least squares plane calculation.

Table 15. Selected Distances (Å) in *trans*-[RhCl(CO)(DPM)]<sub>2</sub>Bonded

Rh-Cl	2.3875 (9)	P(1)-C(11)	1.833 (2)
Rh-P(1)	2.3141 (9)	P(1)-C(21)	1.831 (2)
Rh-P(2) <sup>a</sup>	2.3315 (9)	P(2)-C(31)	1.834 (2)
Rh-C(1)	1.814 (4)	P(2)-C(41)	1.842 (2)
P(1)-C(2)	1.840 (3)	C(1)-O	1.102 (5)
P(2)-C(2)	1.835 (3)		

Nonbonded

Rh-Rh <sup>a</sup>	3.2386 (5)	O-H(14) <sup>c</sup>	2.56
Rh-Cl <sup>a</sup>	3.569 (1)	C(1)-H(16)	2.69
P(1)-P(2)	3.130 (1)	C(2)-H(42)	2.57
Cl-H(16)	2.69	C(2)-H(22)	2.64
Cl-H(45) <sup>b</sup>	2.73		

<sup>a</sup>Primed atoms related to unprimed atoms by a center of inversion in this and all subsequent tables.

<sup>b</sup>Atom located at  $\bar{x}, \bar{y}, 1-z$ .

<sup>c</sup>Atom located at  $x, y-1, z$ .

Table 16. Selected Angles (deg) in *trans*-[RhCl(CO)(DPM)]<sub>2</sub>Bond Angles

Cl-Rh-P(1)	86.20(3)	C(2)-P(1)-C(11)	102.7(1)
Cl-Rh-P(2)	95.33(3)	C(2)-P(1)-C(21)	103.2(1)
Cl-Rh-C(1)	169.1(1)	C(2)-P(2)-C(31)	107.8(1)
C(1)-Rh-P(1)	91.6(1)	C(2)-P(2)-C(41)	101.8(1)
C(1)-Rh-P(2)	87.5(1)	C(11)-P(1)-C(21)	103.1(1)
P(1)-Rh-P(2)	176.50(2)	C(31)-P(2)-C(41)	99.5(1)
Rh-C(1)-O	176.3(4)	P(1)-C(11)-C(12)	121.0(1)
P(1)-C(2)-P(2)	116.8(2)	P(1)-C(11)-C(16)	118.9(1)
Rh-P(1)-C(2)	112.2(1)	P(1)-C(21)-C(22)	122.8(1)
Rh-P(2)-C(2)	110.9(1)	P(1)-C(21)-C(26)	117.1(1)
Rh-P(1)-C(11)	121.22(8)	P(2)-C(31)-C(32)	117.3(1)
Rh-P(1)-C(21)	112.39(9)	P(2)-C(31)-C(36)	122.4(1)
Rh-P(2)-C(31)	120.35(8)	P(2)-C(41)-C(42)	123.6(1)
Rh-P(2)-C(41)	114.53(9)	P(2)-C(41)-C(46)	116.4(1)

Torsion Angles

P(1)-Rh-Rh'-P(2)	2.19(3)	C(1)-Rh-P(1)-C(2)	140.6(2)
Cl-Rh-P(1)-C(2)	-50.1(1)	C(1)-Rh-P(1)-C(11)	18.9(2)
Cl-Rh-P(1)-C(11)	-171.7(1)	C(1)-Rh-P(1)-C(21)	-103.5(2)
Cl-Rh-P(1)-C(21)	65.74(3)	C(1)-Rh-P(2)-C(2)	-90.8(2)
Cl-Rh-P(2)-C(2)	99.7(1)	C(1)-Rh-P(2)-C(31)	142.2(2)
Cl-Rh-P(2)-C(31)	-27.2(1)	C(1)-Rh-P(2)-C(41)	23.7(2)
Cl-Rh-P(2)-C(41)	-145.73(9)		

Vector-Plane Normal Angles

Rh-Rh', Rh-Cl-P(1)	12.98(2)
Rh-Rh', Rh-C(1)-P(2)	23.6(1)



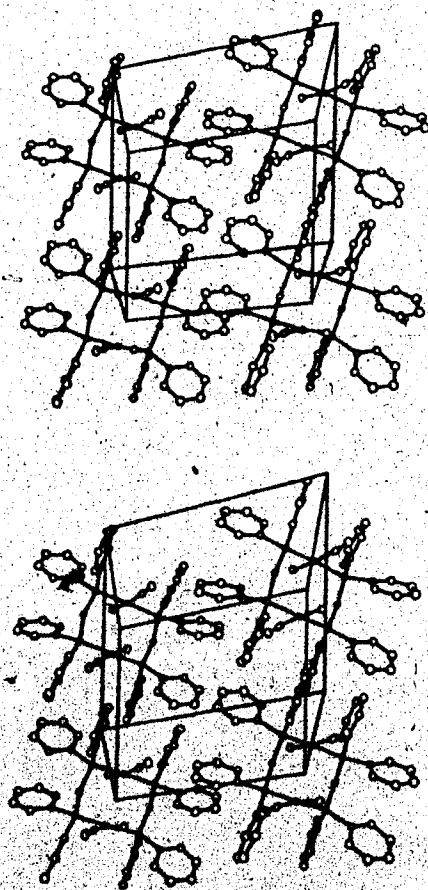


Figure 8. Cell Packing Diagram of *trans*-[RhCl(CO)(DPM)]<sub>2</sub>.

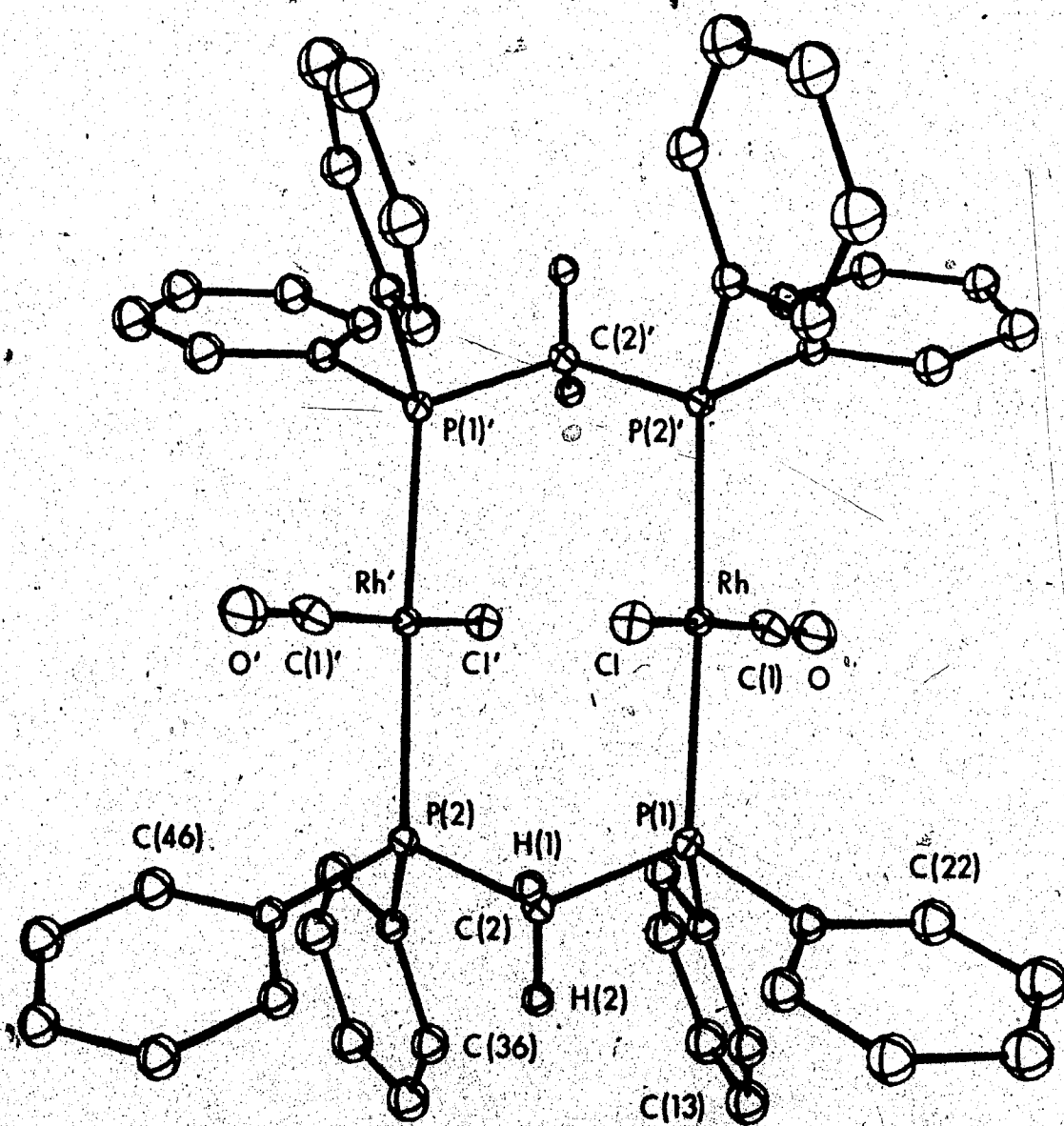


Figure 9. A Perspective View of  $\text{trans-}[\text{RhCl}(\text{CO})(\text{DPM})_2]_2$ .

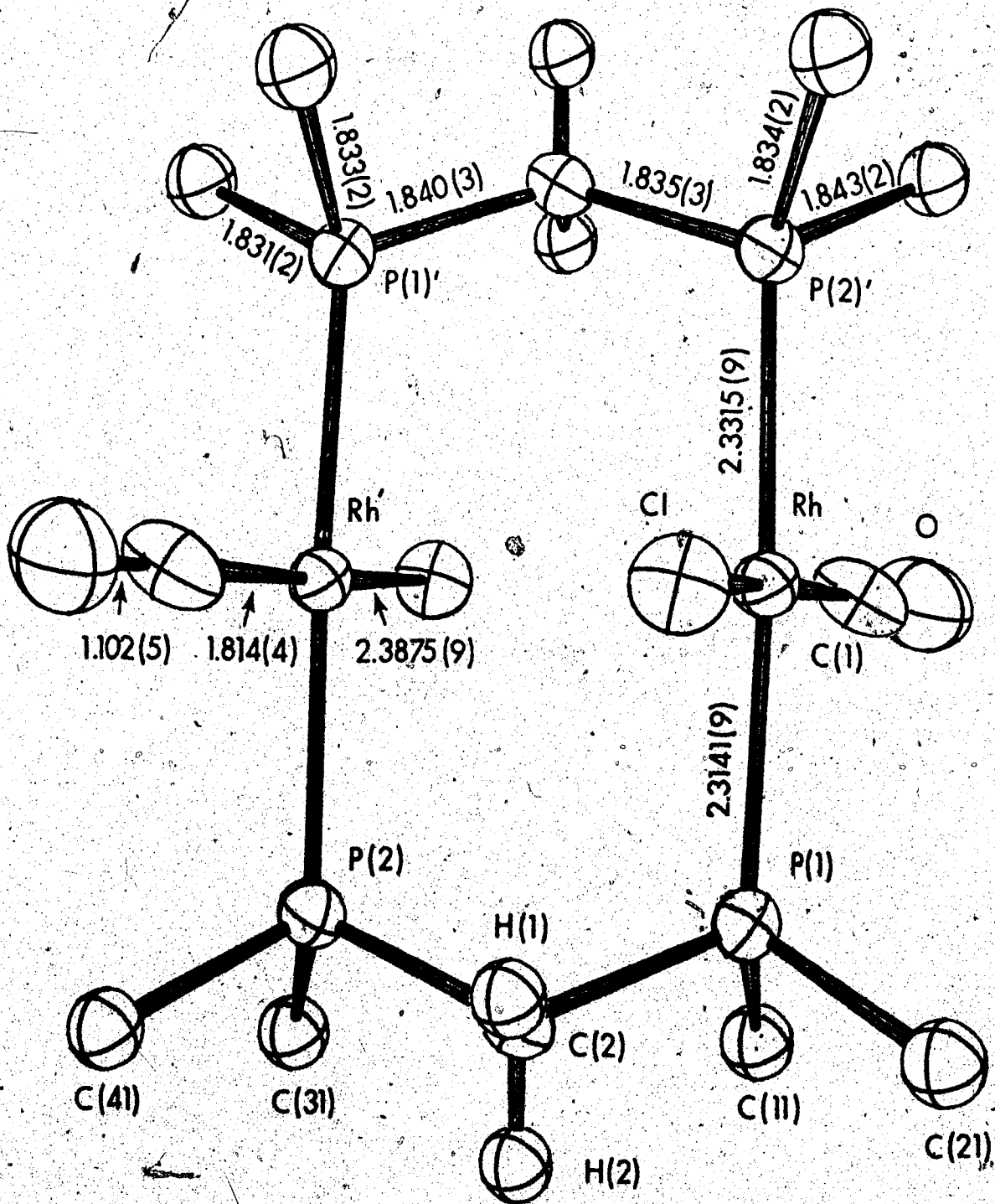


Figure 10. The Inner Coordination Sphere of *trans*-[RhCl(DPM)<sub>2</sub>].

DESCRIPTION OF STRUCTURE

The structure of *trans*-[RhCl(CO)(DPM)]<sub>2</sub> (1) consists of a discrete dimeric unit located on the inversion centre at the origin; thus the molecule possesses crystallographically imposed  $\bar{1}$  symmetry. The coordination about each Rh atom is effectively square planar with *trans* geometry about each metal, much like Vallarino's compound<sup>66</sup> and its analogues.<sup>122</sup> Slight tetrahedral distortions of the square plane are evident as was observed in the red and orange forms of Wilkinson's compound.<sup>117,123</sup> Therefore the two phosphorus atoms are folded towards each other in the direction of the Rh-Rh vector whereas the Cl and CO ligands are folded in the opposite direction (Table 14). The dimeric unit is composed of two of these parallel square planes in an eclipsed conformation and bridged by the diphosphine ligands. These planes are arranged such that the chloro ligands on adjacent rhodium atoms are mutually *trans*, as are the carbonyl ligands. Significantly, the square planes are not perpendicular to the Rh-Rh vector but are inclined to it by *ca.* 75.9° (Table 14) with the chloro ligands folded in towards the bridging sites between the metal centers. This same twist of the Rh square planes is also observed in *trans*-[RhCl(CO)(DAM)]<sub>2</sub>, although it was not noted in the original report on this compound.<sup>31</sup> The skewing of these planes seems to result from an attempt to minimize the non-bonded contacts between the equatorial chloro and carbonyl ligands and the phenyl rings. So in the observed

conformation the Rh-Cl and Rh-CO vectors are staggered with respect to the P-C vectors (Table 16).

Within the Rh-DPM framework the parameters are essentially as observed in other similar DPM-bridged complexes.<sup>35,37,84,85,89</sup> The two independent Rh-P distances (2.3141(9) and 2.3315(9)Å) are significantly different, however no chemical significance is attached to this difference. More likely the difference is a consequence of packing considerations (vide infra). Unlike most other DPM-bridged species which have a cis methylene arrangement, the methylene groups in the present compound are folded in a trans configuration with the methylene carbon atoms displaced by 0.720(4)Å from the best intraligand Rh-P-P-Rh planes. The folding of the methylene carbon atoms out of these planes occurs such that the phenyl groups avoid the equatorial ligands.

The parameters involving the chloro- and carbonyl ligands are not unusual, being typical for Rh(I) phosphino complexes.<sup>31,35,89,120,122</sup>

The relatively long Rh...Rh separation of 3.2386(5)Å is consistent with no formal metal-metal bond, and is in fact significantly longer than the non-bonded Rh...Rh separations of 3.1520(8)Å and 3.155(4)Å observed in [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-Cl)(DPM)<sub>2</sub>][BF<sub>4</sub>]<sup>120</sup> (Chapter II) and [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-S)(DPM)<sub>2</sub>],<sup>89</sup> respectively. In these two "A-frame" species the metal centres are held closer than in the present structure owing to the constraints of the bridging

chloro and sulfido ligands, respectively, in the former two species. As in previous determinations in which no metal-metal bond was present the intraligand P...P separation (3.130(1)Å) is significantly less than the Rh...Rh separation. However the Rh...Rh separation is still considerably less than that observed in the DAM analogue (3.396(1)Å),<sup>31</sup> reflecting the differences in bite size of the two ligands. A further indication that the Rh-Rh interaction, in the present compound, is repulsive is seen in a comparison of the P-C-P (116.8(2)°) and As-C-As (113.5(4)°) angles in the DPM and DAM<sup>31</sup> complexes, respectively. The larger P-C-P angle reflects the strain on the DPM ligand as the metal centres are tending apart.

A comparison of the metrical parameters of the DPM and DAM ligands in the present complex and in *trans*-[RhCl(CO)-(DAM)]<sub>2</sub>,<sup>31</sup> respectively, shows the expected trend resulting from the larger covalent radius of As compared to P. Therefore the average P-C<sub>methylene</sub> (1.838(4)Å),<sup>124</sup> P-C<sub>phenyl</sub> (1.835(5)Å) and Rh-P (2.32(1)Å) distances are all significantly less than the corresponding As-C<sub>methylene</sub> (1.97(2)Å), As-C<sub>phenyl</sub> (1.936(9)Å) and Rh-As (2.407(4)Å) distances.

### DISCUSSION

The primary reason for undertaking the structural determination of *trans*-[RhCl(CO)(DPM)]<sub>2</sub> was to permit comparisons between it and the analogous DAM complex<sup>31</sup> in order to gain an understanding of the differences in their

solubilities and chemistries. Based on the packing of the complex, shown in Figure 5, it is not difficult to understand the insolubility of the DPM complex. All the phenyl rings in the lattice have one of essentially two orientations allowing extremely efficient packing of the molecules and efficient stacking of the parallel phenyl rings. However, since the DPM complex turns out to be essentially isostructural with the DAM analogue we find the solubility differences somewhat surprising. It is therefore assumed that the subtle differences resulting from the larger Rh(DAM) framework (vide supra) result in less efficient packing than in the DPM complex. The effect of the larger molecular framework is obvious in the cell parameters which result in unit cell volume of the DAM complex being ca. 4% larger than that of the DPM complex.

As had been expected, the Rh...Rh separation in the DPM complex is significantly shorter than that in the DAM complex. This arises because of the smaller bite of the DPM ligand which holds the metals closer together. It is anticipated that these different ligand bites will have significant effects on the stability of species containing bridging ligands, especially unsupported ligands such as "ketonic" carbonyls. Certainly studies to date do indicate a difference in stability between DPM and DAM "ketonic" carbonyl species. The present structure and that of complex 2 conclusively establish the significantly different effects that the DPM and DAM ligands have in establishing

metal-metal separations, in analogous structures. However, it must be noted that the present structure and that of 2 as determined by Mague<sup>31</sup> reflect only the preferred metal-metal separations of the two ligands under similar conditions. These ligands have extremely flexible bites which are rather easily changed. Therefore, a redetermination of the structure of *trans*-[RhCl(CO)(DAM)]<sub>2</sub>,<sup>125</sup> as the CH<sub>2</sub>Cl<sub>2</sub> solvate, indicates a Rh-Rh separation of only 3.236(2)Å. This is of course comparable to that in the present DPM compound and much less than that observed in the identical unsolvated complex. The difference (0.160(2)Å) is due presumably to packing considerations. At the other extreme, the largest metal-metal separation of 3.492(1)Å, has been observed in [Pd<sub>2</sub>Cl<sub>2</sub>(μ-HFB)(DPM)<sub>2</sub>],<sup>87</sup> indicating just how far the metals can be forced apart. Notwithstanding, the minimum and maximum metal-metal separations allowed should occur in DPM and DAM, respectively, as is the case for the two essentially isostructural compounds 1 and 2.



## CHAPTER IV.

### The Chemistry of Binuclear Rhodium Complexes with Sulfur Dioxide and the Structure of $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]^+$

#### INTRODUCTION

The cationic "A-frame" species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  (1) has been shown to undergo facile and often reversible reactions with small molecules.<sup>35a,91,96a</sup> An X-ray structural determination of 1 as the  $\text{BF}_4^-$  salt has indicated that both the enclosed bridging site, between the metal centres, and the terminal exposed sites, remote from the bridging site, are open to attack by small molecules<sup>120</sup> (Chapter II). The accessibility of these sites has been confirmed by experiments which have shown that CO attacks at the terminal site,<sup>91</sup> yielding  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2]^+$  (2) (see Figure 11), whereas preliminary studies indicated that attack by  $\text{SO}_2$  seems to occur directly at the bridging site.<sup>96a</sup> Therefore a detailed study of the chemistry of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  with  $\text{SO}_2$  was undertaken to gain a better understanding of the modes of  $\text{SO}_2$  attack and coordination.

It was also observed that on prolonged treatment of the initially formed adduct  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\mu\text{-SO}_2)(\text{DPM})_2]^+$  (3) with  $\text{SO}_2$ , a disproportionation reaction seemed to occur yielding a neutral carbonyl free species containing  $\text{SO}_2$ , which was formulated as  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  (4), and at



least one other unidentified species (5).<sup>96a</sup> The structural characterization of this new SO<sub>2</sub> complex was undertaken to establish unambiguously its identity and a detailed investigation of the chemistry yielding the species was undertaken to establish the nature of this "disproportionation" reaction.

In addition the chemistry of another binuclear complex, *trans*-[RhCl(CO)(DPM)]<sub>2</sub>, with SO<sub>2</sub> was investigated to offer comparisons with the chemistry of the "A-frame" species (1). In the dichlorodicarbonyl species only terminal attack is possible, since the positions between the metal centres are blocked by the equatorial ligands<sup>126</sup> (Chapter III). Therefore, interesting comparisons in the chemistries of this species with that of the "A-frame" complex (1) were anticipated.

### EXPERIMENTAL

#### Preparation of [Rh<sub>2</sub>Cl<sub>2</sub>(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>], Method A

A solution of 0.100 g (0.072 mmol) of [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-Cl)(DPM)<sub>2</sub>][BPh<sub>4</sub>] in 10 mL of THF was treated with SO<sub>2</sub> for 10 min and then crystallization was induced by addition of diethyl ether saturated with SO<sub>2</sub>. The resulting red orange crystals, analyzed as [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-Cl)(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>][BPh<sub>4</sub>] (3a) and were obtained in 90-95% yield. This solid was re-dissolved in THF and slow concentration under a stream of SO<sub>2</sub> yielded the final product, [Rh<sub>2</sub>Cl<sub>2</sub>(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>], 4, as well formed red-orange crystals. The remaining solution

was yellow. The yield of this second  $\text{SO}_2$  complex varied between 0 and 50%, depending on the batch of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$  used (vide infra). Elemental analyses for all complexes are shown in Table 17 and the spectroscopic data and conductivity measurements are given in Table 18.

#### Method B

A suspension of 0.200 g (0.182 mmol) of *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$ <sup>66</sup> in 20 mL of  $\text{CH}_2\text{Cl}_2$  was treated with  $\text{SO}_2$  for approximately 2 h. Slow concentration, under a stream of  $\text{SO}_2$ , yielded the desired crystalline product in 95% yield.

#### Method C

To a solution of 0.100 g (0.202 mmol) of  $[\text{RhCl}(\text{COD})]_2$ <sup>99</sup> in 20 mL of  $\text{CH}_2\text{Cl}_2$  was added 0.156 g (0.405 mmol) of DPM dissolved in 5 mL of benzene. Immediate treatment with  $\text{SO}_2$  and concentration of the solution by evaporation under  $\text{SO}_2$  yielded the crystalline product  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  in 90% yield.

#### Preparation of $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{Cl}]$ , $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{Cl}]$ and *cis*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$

Treatment of a solution of 0.100 g (0.085 mmol) of  $[\text{Rh}_2\text{Cl}_2(\text{SO}_2)(\text{DPM})_2]$  in 10 mL of  $\text{CH}_2\text{Cl}_2$  with CO and concentration under a CO stream yielded quantitatively the product  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{Cl}]$  (2b) as an orange microcrystalline solid. Pumping on this solid under vacuum resulted in the total conversion of 2b to  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})-$

Table 17. Analytical Data on Complexes

No.	Complex	Found	Calculated
2b.	$[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{Cl}]$	C, 56.39; H, 4.25; Cl, 6.43	C, 56.36; H, 3.93; Cl, 6.28
3a.	$[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\mu\text{-SO}_2)(\text{DPM})_2][\text{BPh}_4]$	C, 62.85; H, 4.44	C, 62.98; H, 4.45
3b.	$[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\mu\text{-SO}_2)(\text{DPM})_2][\text{Cl}]$	C, 53.01; H, 4.09	C, 53.58; H, 3.80
4.	$[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$	C, 54.6; H, 3.80	C, 54.12; H, 4.00
6.	$\text{cis-}[\text{Rh}_2\text{Cl}_2(\text{CO})_2(\text{DPM})_2]$	C, 57.37; H, 4.55; Cl, 6.46	C, 56.70; H, 4.03; Cl, 6.44

Table 18. Spectral and Conductivity Data on the Complexes

No.	Complex	Infrared Absorption Maxima <sup>a</sup>	Assignment	<sup>31</sup> P{ <sup>1</sup> H}nmr Chemical Shifts <sup>b</sup>	Conductivity <sup>c</sup> (ohm <sup>-1</sup> cm <sup>2</sup> mole <sup>-1</sup> )
1a.	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-Cl)(DPM) <sub>2</sub> ][BPh <sub>4</sub> ] <sup>d</sup>	1997(s), 1978(vs) <sup>e</sup>	νCO	16.1 (113.3 Hz)	99.0
1b.	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-Cl)(DPM) <sub>2</sub> ][Cl]	1994(s), 1972(vs)	νCO	--	--
2a.	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-CO)(μ-Cl)(DPM) <sub>2</sub> ][BPh <sub>4</sub> ] <sup>d</sup>	1992(s), 1977(vs), 1863(s)	νCO	29.6 (94.2 Hz)	94.0
2b.	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-CO)(μ-Cl)(DPM) <sub>2</sub> ][Cl]	2004(s), 1960(vs), 1868(s)	νCO	29.8 (94.0 Hz)	115.0 (acetone) 49.6 (CH <sub>2</sub> Cl <sub>2</sub> )
3a.	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-Cl)(μ-SO <sub>2</sub> )(DPM) <sub>2</sub> ][BPh <sub>4</sub> ]	2015(s), 1985(ssh)	νCO	24.6 (91.3 Hz)	90.0
		1229(m), 1070(m)	νSO <sub>2</sub>		
3b.	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-Cl)(μ-SO <sub>2</sub> )(DPM) <sub>2</sub> ][Cl]	2010(s), 1985(ssh)	νCO	24.5 (91.6 Hz)	65.0
		1230(m), 1071(m)	νSO <sub>2</sub>		
4.	[Rh <sub>2</sub> Cl <sub>2</sub> (μ-SO <sub>2</sub> )(DPM) <sub>2</sub> ]	1191(m), 1063(m)	νSO <sub>2</sub>	19.6 (115.0 Hz)	0
5.	cis-[Rh <sub>2</sub> Cl <sub>2</sub> (CO) <sub>2</sub> (DPM) <sub>2</sub> ]	1971(s)	νCO	19.6 (113.5 Hz)	0
7.	trans-[Rh <sub>2</sub> Cl <sub>2</sub> (CO) <sub>2</sub> (DPM) <sub>2</sub> ] <sup>e</sup>	1968(s)	νCO		0

<sup>a</sup>Infrared spectra were run as Nujol Mulls on-KBr Plates; vs, very strong; s, strong; m, medium; w, weak; sh, shoulder.

<sup>b</sup><sup>31</sup>P{<sup>1</sup>H}nmr chemical shifts are relative to H<sub>3</sub>PO<sub>4</sub> (down field positive), coupling constants (<sup>1</sup>J<sub>Rh-P</sub> + x J<sub>Rh-P</sub>) are given in parentheses.

<sup>c</sup>Solvent is acetone unless noted otherwise.

<sup>d</sup>References 35 and 91.

<sup>e</sup>Reference 66.

(DPM)<sub>2</sub>]Cl] (1b). Bubbling dinitrogen through the solution of 2b followed by slow concentration under dinitrogen yielded "*cis*-[RhCl(CO)(DPM)]<sub>2</sub>" 6 as a yellow crystalline solid.

#### Spectroscopic Studies on the Stepwise Reactions with SO<sub>2</sub>

A solution was prepared by dissolving 0.100 g (0.072 mmol) of 1a in 3 mL of CD<sub>2</sub>Cl<sub>2</sub> in a 10 mm NMR tube. This was cooled in a 2-propanol/dry ice bath and approximately 0.5 mL of gaseous SO<sub>2</sub> was admitted. The <sup>31</sup>P{<sup>1</sup>H} NMR spectrum was recorded immediately at 223 K. This procedure was repeated measuring the NMR spectrum after each addition of SO<sub>2</sub> until nearly all of 1a had been converted to 3a. Throughout the experiment only resonances assignable to 1a or 3a were detected.

Infrared spectra were recorded in an analogous manner, by recording the infrared spectrum after each stepwise addition of 0.5 ml of SO<sub>2</sub> (at atmospheric pressure) to a CH<sub>2</sub>Cl<sub>2</sub> solution of 1a (0.500 g (0.361 mmol) in 30 mL). Only bands assignable to complexes 1a, 3a and free SO<sub>2</sub> were detected. The stepwise addition of SO<sub>2</sub> to *trans*-[RhCl(CO)(DPM)]<sub>2</sub> was similarly monitored by infrared spectroscopy; however, in this case infrared bands at 1740(m), 1995(sh) and 2020(s) cm<sup>-1</sup> were observed at intermediate times in the experiment. After all of the *trans*-dichlorodicarbonyl complex had reacted, only bands attributable to 3b and free SO<sub>2</sub> were observed (Table 18). The NMR and infrared studies on both complexes indicated

that several additions of  $\text{SO}_2$  were required before any evidence of a reaction was detected.

A  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of a sample of 3a that had "disproportionated" showed bands assignable to 3a and 4 as well as bands at  $\delta = 8.05$  ppm (singlet),  $^{101}\delta = 5.90$  ppm (doublet, 70 Hz) and  $\delta = -13.4$  ppm (doublet, 120 Hz). The sum of the integrated intensities of the last three peaks was approximately equal to that of 4.

#### X-ray Data Collection

Red crystals of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  suitable for single-crystal X-ray diffraction studies, were supplied by Dr. A.R. Sanger of the Alberta Research Council. Preliminary film data showed that the crystals belonged to the monoclinic system with extinctions ( $h0l, l \text{ odd}; 0k0, k \text{ odd}$ ) characteristic of the centrosymmetric space group  $\text{P}2_1/c$ . See Table 19 for pertinent crystal data and intensity collection information and Chapter II for a more complete discussion of data collection.

#### Structure Solution and Refinement

The structure was solved by using a sharpened Patterson map to locate the two independent Rh atoms. Subsequent refinements and electron density difference maps led to the location of all remaining atoms. Anomalous dispersion terms<sup>108</sup> for Rh, P, Cl and S were included in  $F_c$ . The phenyl rings were refined as rigid groups and the hydrogen atoms were included as fixed contributions and not refined.



Table 19. Summary of Crystal Data and Intensity Collection

for  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$ 

Compound	$[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$																																
Formula	$\text{C}_{50}\text{H}_{44}\text{Cl}_2\text{O}_2\text{P}_4\text{Rh}_2\text{S}$																																
Formula Weight	1109.58 amu																																
Cell Parameters																																	
a	18.228(1) Å																																
b	13.526(1) Å																																
c	19.632(2) Å																																
$\beta$	104.72(1)°																																
V	4681.6 Å <sup>3</sup>																																
Z	4																																
Density	1.574 g·cm <sup>-3</sup> (calc'd.) 1.59(2) g·cm <sup>-3</sup> (expt'l. by flotation)																																
Space Group	$\text{C}_{2h}^5 = \text{P2}_1/\text{c}$																																
Crystal Dimensions	0.31 x 0.21 x 0.06 mm																																
Crystal Volume	0.0025 mm <sup>3</sup>																																
Crystal Faces (and distances from an arbitrary origin within the crystal (mm))	<table border="1"> <tbody> <tr><td><math>\bar{1}</math></td><td>0</td><td>0</td><td>(0.0213)</td></tr> <tr><td><math>\bar{1}</math></td><td>0</td><td>0</td><td>(0.0194)</td></tr> <tr><td>0</td><td>0</td><td><math>\bar{1}</math></td><td>(0.1470)</td></tr> <tr><td>0</td><td>0</td><td><math>\bar{1}</math></td><td>(0.1460)</td></tr> <tr><td><math>\bar{1}</math></td><td><math>\bar{1}</math></td><td>0</td><td>(0.0913)</td></tr> <tr><td><math>\bar{1}</math></td><td><math>\bar{1}</math></td><td>0</td><td>(0.0810)</td></tr> <tr><td><math>\bar{1}</math></td><td><math>\bar{1}</math></td><td>0</td><td>(0.0790)</td></tr> <tr><td><math>\bar{1}</math></td><td><math>\bar{1}</math></td><td>0</td><td>(0.0940)</td></tr> </tbody> </table>	$\bar{1}$	0	0	(0.0213)	$\bar{1}$	0	0	(0.0194)	0	0	$\bar{1}$	(0.1470)	0	0	$\bar{1}$	(0.1460)	$\bar{1}$	$\bar{1}$	0	(0.0913)	$\bar{1}$	$\bar{1}$	0	(0.0810)	$\bar{1}$	$\bar{1}$	0	(0.0790)	$\bar{1}$	$\bar{1}$	0	(0.0940)
$\bar{1}$	0	0	(0.0213)																														
$\bar{1}$	0	0	(0.0194)																														
0	0	$\bar{1}$	(0.1470)																														
0	0	$\bar{1}$	(0.1460)																														
$\bar{1}$	$\bar{1}$	0	(0.0913)																														
$\bar{1}$	$\bar{1}$	0	(0.0810)																														
$\bar{1}$	$\bar{1}$	0	(0.0790)																														
$\bar{1}$	$\bar{1}$	0	(0.0940)																														
Temperature	20°C																																
Radiation	CuK $\alpha$ ( $\lambda=1.540562$ Å) filtered with 0.5 mil thick nickel foil																																
$\mu$	89.55 cm <sup>-1</sup>																																
Range in Absorption Correction Factors	0.229 - 0.700																																
Receiving Aperture	3x3 mm, 30 cm from the crystal																																
Takeoff Angle	2.6°																																

Table 19, continued

Scan Speed	2° in 2θ/min (3° < 2θ < 100°)
Scan Range	1° in 2θ/min (100° < 2θ < 123°) 0.75° below K <sub>α1</sub> to 0.75° above K <sub>α2</sub>
Background Counting Time	10s (3° < 2θ < 76°) 20s (76° < 2θ < 100°) 40s (100° < 2θ < 123°)
2θ limits	3° < 2θ < 123°
2θ units for centred reflections	50° < 2θ < 70°
Final number of variables	216
Unique Data Collected	7690
Unique Data Used (F <sub>o</sub> <sup>2</sup> ≥ 3σ(F <sub>o</sub> <sup>2</sup> ))	5207
Error in observation of unit weight	2.199
R	0.058
R <sub>w</sub>	0.067

All nongroup atoms were refined individually with anisotropic thermal parameters. An isotropic secondary extinction parameter was included and refined since several intense low angle reflections systematically showed  $F_{obs}$  significantly less than  $F_{cal}$ .<sup>92</sup> (For a more detailed discussion of the techniques used in solution of the structure see Chapter II.)

The final model with 216 parameters varied converged to  $R = 0.058$  and  $R_w = 0.067$ .<sup>121</sup> In the final electron density difference map all of the 20 highest residuals were in the vicinities of the phenyl groups ( $0.99-0.55 e/\text{\AA}^3$ ). A typical carbon atom on an earlier synthesis had an electron density of about  $3.9 e/\text{\AA}^3$ .

On the basis of the high thermal parameters of some of these group atoms and the residuals about the phenyl groups, it seems that an anisotropic refinement of the phenyl carbon atoms would have been more suitable. However this was not attempted due to the very high cost and the feeling that no significant change would result in the parameters of interest.

### Results

The positional and thermal parameters for the individual anisotropic atoms, rigid group atoms and idealized hydrogen atoms are given in Tables 20, 21 and 22, respectively. Least-squares plane calculations are shown in Table 23 and selected bond lengths and angles are given in Tables 24

and 25, respectively. A listing of the observed and calculated structure amplitudes is available.<sup>110</sup>

A stereoview of the unit cell is shown in Figure 12. The crystallographic *a* axis is horizontal to the right, the *c* axis runs from top to bottom and the *b* axis goes into the page. Figure 13 presents a perspective view of the compound including the numbering scheme (phenyl hydrogen atoms have the same number as their attached carbon atom). The inner coordination sphere is shown in Figure 14 along with some relevant bond lengths, 50% thermal ellipsoids are drawn.

TABLE 20. Positional and Thermal Parameters For The Nongroup Atoms of [Rh2C12(mu-SO2)(DPM)2].

Atom	x <sup>a</sup>	y	z	U11	U22	U33	U12	U13	U23
Rh(1)	0.27944(3)	0.38834(5)	0.51141(3)	3.61(4)	3.37(4)	3.52(4)	-0.11(3)	1.37(3)	0.04(3)
Rh(2)	0.21069(3)	0.16337(5)	0.45320(3)	3.41(4)	3.65(4)	2.77(4)	0.05(3)	0.85(3)	-0.10(3)
P(1)	0.1677(1)	0.4272(2)	0.5018(1)	4.1(1)	3.8(1)	3.7(1)	0.2(1)	1.6(1)	0.2(1)
P(2)	0.0937(1)	0.2442(2)	0.4266(1)	3.3(1)	4.2(1)	3.2(1)	-0.1(1)	1.07(9)	0.0(1)
P(3)	0.3957(1)	0.2738(2)	0.5056(1)	3.7(1)	4.0(1)	4.8(1)	-0.1(1)	1.6(1)	0.1(1)
P(4)	0.3232(1)	0.0771(2)	0.4579(1)	4.2(1)	4.1(1)	3.9(1)	0.9(1)	0.5(1)	-0.4(1)
C1(1)	0.3413(1)	0.4912(2)	0.5333(2)	5.2(1)	4.0(1)	8.2(2)	-0.7(1)	1.3(1)	-0.3(1)
C1(2)	0.1495(1)	0.0353(2)	0.3805(1)	4.8(1)	4.8(1)	4.3(1)	-1.0(1)	1.2(1)	-1.1(1)
S	0.2441(1)	0.2110(2)	0.5622(1)	4.1(1)	3.8(1)	2.8(1)	-0.11(9)	1.10(9)	0.09(9)
O(1)	0.3057(4)	0.1574(5)	0.6091(3)	5.2(4)	5.3(4)	3.2(3)	0.7(3)	0.4(3)	0.9(3)
O(2)	0.1805(3)	0.2256(5)	0.5932(3)	4.9(4)	5.6(4)	3.4(3)	0.3(3)	2.4(3)	0.7(3)
C(1)	0.0830(5)	0.3497(6)	0.4814(5)	3.5(4)	4.2(5)	3.9(5)	0.4(4)	1.3(4)	0.4(4)
C(2)	0.4077(5)	0.1385(6)	0.5106(5)	4.1(5)	4.5(5)	4.4(6)	0.3(4)	1.0(4)	0.2(4)

<sup>a</sup> Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

<sup>b</sup> The form of the thermal ellipsoid is:  $\exp[-2\pi i(a^*U_{11}h^2 + b^*U_{22}k^2 + c^*U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl)]$ . The quantities given in the table are the thermal coefficients  $\times 10^4$ .

TABLE 21. Derived Parameters For the Rigid Group Atoms of [Rh2C12(mu-SO2)(DPM)2].

Atom	X	Y	Z	B(A <sup>1</sup> )	Atom	X	Y	Z	B(A <sup>1</sup> )
C(11)	0.1471(6)	0.5213(5)	0.4326(5)	3.4(2)	C(51)	0.4781(9)	0.3152(7)	0.5723(4)	3.7(2)
C(12)	0.1927(5)	0.5318(5)	0.3860(4)	4.7(2)	C(52)	0.531(7)	0.3813(7)	0.5592(7)	7.0(3)
C(13)	0.1763(7)	0.6044(6)	0.3341(4)	6.1(3)	C(53)	0.5924(6)	0.4107(5)	0.6138(8)	8.1(4)
C(14)	0.1142(6)	0.6666(5)	0.3288(5)	6.3(3)	C(54)	0.6001(9)	0.3740(7)	0.6815(4)	7.3(3)
C(15)	0.0686(5)	0.6561(5)	0.3755(4)	7.9(4)	C(55)	0.547(1)	0.3079(7)	0.6946(7)	12.3(6)
C(16)	0.0850(7)	0.5835(6)	0.4274(4)	6.6(3)	C(56)	0.4857(6)	0.2785(5)	0.6400(8)	9.7(5)
C(21)	0.1620(5)	0.4948(5)	0.5809(3)	3.7(2)	C(61)	0.408(2)	0.3061(6)	0.419(1)	4.3(2)
C(22)	0.1879(5)	0.5919(5)	0.5907(3)	5.9(3)	C(62)	0.478(1)	0.3022(5)	0.4032(9)	8.3(4)
C(23)	0.1933(4)	0.6390(4)	0.6548(4)	6.3(3)	C(63)	0.483(2)	0.3235(6)	0.335(1)	10.2(5)
C(24)	0.1726(5)	0.5892(5)	0.7091(3)	6.1(3)	C(64)	0.419(2)	0.3488(6)	0.283(1)	7.8(4)
C(25)	0.1467(5)	0.4921(5)	0.6994(3)	5.6(3)	C(65)	0.348(1)	0.3527(5)	0.2994(9)	6.3(3)
C(26)	0.1413(4)	0.4450(4)	0.6353(4)	4.5(2)	C(66)	0.343(2)	0.3314(6)	0.367(1)	4.5(2)
C(31)	0.0089(4)	0.1740(4)	0.429(1)	3.1(2)	C(71)	0.349(1)	0.0554(7)	0.3747(5)	4.6(2)
C(32)	-0.0037(9)	0.1526(6)	0.4941(6)	5.9(3)	C(72)	0.4136(9)	0.0005(6)	0.3759(8)	11.5(6)
C(33)	-0.069(1)	0.1015(6)	0.4982(6)	7.6(4)	C(73)	0.4372(5)	-0.0123(6)	0.3144(9)	14.8(7)
C(34)	-0.1211(4)	0.0718(4)	0.437(1)	5.8(3)	C(74)	0.396(1)	0.0298(7)	0.2516(5)	8.7(4)
C(35)	-0.1086(9)	0.0932(6)	0.3715(6)	6.0(3)	C(75)	0.3309(9)	0.0846(6)	0.2504(8)	6.0(3)
C(36)	-0.044(1)	0.1443(6)	0.3673(6)	5.4(3)	C(76)	0.3073(5)	0.0974(6)	0.3119(9)	4.6(2)
C(41)	0.0776(6)	0.2969(5)	0.3383(5)	3.1(2)	C(81)	0.3265(5)	-0.0469(5)	0.4969(5)	4.0(2)
C(42)	0.0170(5)	0.3601(5)	0.3109(4)	5.0(2)	C(82)	0.3470(5)	-0.0588(5)	0.5698(5)	5.6(3)
C(43)	0.0079(4)	0.4008(4)	0.2441(6)	6.0(3)	C(83)	0.3457(5)	-0.1523(7)	0.5990(3)	6.7(3)
C(44)	0.0594(6)	0.3784(5)	0.2048(5)	5.2(2)	C(84)	0.3238(5)	-0.2340(5)	0.5553(5)	6.5(3)
C(45)	0.1200(5)	0.3152(5)	0.2322(4)	5.2(2)	C(85)	0.3033(5)	0.2220(5)	0.4825(5)	9.0(4)
C(46)	0.1291(4)	0.2745(4)	0.2990(6)	4.1(2)	C(86)	0.3046(5)	-0.1285(7)	0.4533(3)	8.6(4)

Rigid Group Parameters

	Xc	Yc	Zc	Delta	Epsilon	Eta
Ring1	0.1306(3)	0.5939(4)	0.3807(3)	-0.703(4)	0.864(7)	4.322(6)
Ring2	0.1673(2)	0.5420(4)	0.6450(3)	0.339(5)	1.464(5)	5.775(5)
Ring3	-0.0561(3)	0.1229(3)	0.4328(3)	1.049(4)	1.79(1)	1.48(1)
Ring4	0.0685(3)	0.3376(3)	0.2715(3)	2.242(4)	1.124(7)	2.452(7)
Ring5	0.5391(3)	0.3446(4)	0.6269(3)	0.872(6)	2.146(8)	5.824(9)
Ring6	0.4133(3)	0.3274(3)	0.3513(3)	-1.303(5)	0.62(2)	4.04(2)
Ring7	0.3722(3)	0.0426(4)	0.3132(4)	-0.980(6)	1.45(1)	2.92(1)
Ring8	0.3252(3)	-0.1404(4)	0.5261(3)	0.144(5)	1.853(5)	1.165(5)

a Xc, Yc and Zc are the fractional coordinates of the centroid of the rigid group.  
 b The rigid group orientation angles Delta, Epsilon and Eta (radians) are the angles by which the rigid body is rotated with respect to a set of axes X, Y and Z. The origin is the centre of the ring; X is parallel to a\*, Z is parallel to c, and Y is parallel to the line defined by the intersection of the plane containing a\* and b\*.

TABLE 22. Idealized Positional and Thermal Parameters For the Hydrogen Atoms of [Rh2C12(mu-SO2)(DPM)2].

Atom	x	y	z	B(A <sup>2</sup> )	Atom	x	y	z	B(A <sup>2</sup> )
H(1C1)	0.0409	0.3882	0.4571	3.99	H(45)	0.1552	0.2998	0.2054	6.20
H(2C1)	0.0739	0.3262	0.5241	3.99	H(46)	0.1705	0.2313	0.3477	5.09
H(1C2)	0.4163	0.1179	0.5583	4.43	H(52)	0.5261	0.4064	0.5129	7.98
H(2C2)	0.4502	0.1205	0.4937	4.43	H(53)	0.6288	0.4559	0.6048	9.09
H(12)	0.2351	0.4894	0.3896	5.72	H(54)	0.6416	0.3941	0.7187	8.29
H(13)	0.2075	0.6116	0.3023	7.13	H(55)	0.5519	0.2829	0.7407	13.27
H(14)	0.1030	0.7161	0.2934	7.33	H(56)	0.4493	0.2334	0.6489	10.73
H(15)	0.0262	0.6985	0.3718	8.93	H(62)	0.5221	0.2846	0.4387	9.35
H(16)	0.0538	0.5763	0.4591	7.59	H(63)	0.5311	0.3206	0.3245	11.11
H(22)	0.2020	0.6259	0.5536	6.84	H(64)	0.4222	0.3633	0.2371	8.82
H(23)	0.2110	0.7052	0.6615	7.20	H(65)	0.3043	0.3701	0.2640	7.29
H(24)	0.1763	0.6212	0.7529	7.10	H(66)	0.2953	0.3341	0.3783	5.52
H(25)	0.1326	0.4579	0.7364	6.60	H(72)	0.4417	-0.0280	0.4190	12.62
H(26)	0.1236	0.3786	0.6286	5.55	H(73)	0.4815	-0.0497	0.3155	15.60
H(32)	0.0321	0.1729	0.5359	6.91	H(74)	0.4121	0.0209	0.2099	9.66
H(33)	-0.0773	0.0869	0.5428	8.60	H(75)	0.3028	0.1133	0.2076	7.05
H(34)	-0.1655	0.0370	0.4397	6.77	H(76)	0.2629	0.1350	0.3110	5.64
H(35)	-0.1442	0.0730	0.3296	5.98	H(82)	0.3620	-0.0030	0.5996	6.57
H(36)	-0.0349	0.1590	0.3226	6.43	H(83)	0.3597	-0.1604	0.6487	7.68
H(42)	-0.0181	0.3754	0.3377	6.03	H(84)	0.3229	-0.2977	0.5753	7.51
H(43)	-0.0334	0.4439	0.2254	6.96	H(85)	0.2883	-0.2775	0.4527	10.05
H(44)	0.0533	0.4061	0.1593	6.20	H(86)	0.2906	-0.1201	0.4037	9.60

Table 23. Least-Squares Plane Calculations

Plane No.	Equation <sup>a</sup>
1	$0.2235 X + 0.3314 Y - 0.9166 Z + 6.7751 = 0.0$
2	$-0.9043 X + 0.4149 Y - 0.1006 Z + 1.3775 = 0.0$
3	$-0.3075 X - 0.8651 Y - 0.3962 Z + 7.2045 = 0.0$

Deviation from Planes (Å)

Atom

Plane No.	Rh(1)	Rh(2)	P(1)	P(2)	P(3)	P(4)	C(1)	C(2)	S	O(1)	O(2)
1	-0.0407(6)	-0.0272(6)	0.081(2)	0.352(2)	0.250(2)	0.250(2)	-0.234(9) <sup>b</sup>	-0.400(9) <sup>b</sup>			
2	0.0	0.0							0.0		
3									0.0	0.0	0.0

Dihedral Angle Between Planes 2 and 3 = 92.35°

<sup>a</sup>X, Y, Z are the orthogonal coordinates (Å) with X along the a axis, Y in the a-b plane and Z along the c\* axis.

<sup>b</sup>Not included in least squares plane calculations.



Table 24. Selected Distances  $\dagger$ (Å) in  $\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2$ 

Bond Distances			
Rh(1)-Rh(2)	2.7838(8)		
Rh(1)-S	2.169(2)		
Rh(2)-S	2.169(2)		
Rh(1)-Cl(1)	2.342(2)		
Rh(2)-Cl(2)	2.341(2)		
Rh(1)-P(1)	2.330(2)	2.331(9) <sup>a</sup>	
Rh(1)-P(3)	2.320(2)		
Rh(2)-P(2)	2.334(2)		
Rh(2)-P(4)	2.341(2)		
S-O(1)	1.452(6)		
S-O(2)	1.452(6)		
		P(1)-C(1)	1.824(9)
		P(2)-C(1)	1.827(9)
		P(3)-C(2)	1.843(9)
		P(4)-C(2)	1.822(9)
		P(1)-C(11)	1.830(6)
		P(1)-C(21)	1.830(6)
		P(2)-C(31)	1.824(5)
		P(2)-C(41)	1.827(5)
		P(3)-C(51)	1.812(7)
		P(3)-C(61)	1.820(7)
		P(4)-C(71)	1.832(7)
		P(4)-C(81)	1.839(6)

1.829(9)

1.827(8)

## Nonbonded Distances

P(1)-P(2)	3.018(3)	O(1)-H1C2 <sup>b</sup>	2.52
P(3)-P(4)	3.012(3)	O(2)-H(45)	2.39
Rh(1)-H(66)	2.70	O(2)-H2C1	2.48
Rh(2)-H(46)	2.73	O(2)-H(26)	2.49
C(52)-H(62)	2.67	H2C1-H(26)	2.15
C(62)-H(52)	2.54	H1C2-H(82)	2.17
O(1)-H(82)	2.43	H(46)-H(76)	2.16
		H(52)-H(62)	2.19

<sup>a</sup>For averaged quantities, the estimated standard deviation is the larger of an individual standard deviation or the standard deviation of a single observation as calculated from the mean.

<sup>b</sup>H(45) is associated with the molecule at the general equivalent position  $x, 1/2 - y, 1/2 + z$ .

Table 25. Selected Angles (deg) in  $\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2$ 

## Bond Angles

Rh(2)-Rh(1)-Cl(1)	166.28(8)	Rh(1)-P(3)-C(51)	116.6(3)
Rh(2)-Rh(1)-P(1)	96.43(6)	Rh(1)-P(3)-C(61)	106.6(3)
Rh(2)-Rh(1)-P(3)	88.94(6)	Rh(2)-P(4)-C(71)	117.6(3)
Rh(2)-Rh(1)-S	50.07(6)	Rh(2)-P(4)-C(81)	114.0(3)
Cl(1)-Rh(1)-S	143.33(9)	C(1)-P(1)-C(11)	103.5(4)
Cl(1)-Rh(1)-P(1)	85.98(9)	C(1)-P(1)-C(21)	104.3(4)
Cl(1)-Rh(1)-P(3)	86.45(9)	C(1)-P(2)-C(31)	100.1(4)
P(1)-Rh(1)-P(3)	168.46(9)	C(1)-P(2)-C(41)	103.8(3)
P(1)-Rh(1)-S	95.23(8)	C(2)-P(3)-C(51)	101.7(4)
P(3)-Rh(1)-S	96.04(8)	C(2)-P(3)-C(61)	103.4(4)
Rh(1)-Rh(2)-Cl(2)	167.17(6)	C(2)-P(4)-C(71)	102.2(4)
Rh(1)-Rh(2)-P(2)	89.10(6)	C(2)-P(4)-C(81)	102.2(4)
Rh(1)-Rh(2)-P(4)	96.25(6)	C(11)-P(1)-C(21)	103.7(3)
Rh(1)-Rh(2)-S	50.08(6)	C(31)-P(2)-C(41)	106.9(3)
Cl(2)-Rh(2)-S	142.44(8)	C(51)-P(3)-C(61)	108.9(4)
Cl(2)-Rh(2)-P(2)	86.75(7)	C(71)-P(4)-C(81)	103.7(4)
Cl(2)-Rh(2)-P(4)	86.11(8)	P(1)-C(11)-C(12)	120.9(4)
P(2)-Rh(2)-P(4)	169.59(9)	P(1)-C(11)-C(16)	119.0(4)
P(2)-Rh(2)-S	95.37(8)	P(1)-C(21)-C(22)	119.9(4)
P(4)-Rh(2)-S	94.91(8)	P(1)-C(21)-C(26)	119.6(4)
Rh(1)-S-Rh(2)	79.84(7)	P(2)-C(31)-C(32)	117.9(4)
O(1)-S-O(2)	111.9(4)	P(2)-C(31)-C(36)	122.1(4)
Rh(1)-S-O(1)	114.6(3)	P(2)-C(41)-C(42)	121.8(4)
Rh(1)-S-O(2)	116.5(3)	P(2)-C(41)-C(46)	118.2(4)
Rh(2)-S-O(1)	117.1(3)	P(3)-C(51)-C(52)	123.7(6)
Rh(2)-S-O(2)	113.6(3)	P(3)-C(51)-C(56)	116.3(6)
Rh(1)-P(1)-C(1)	113.3(3)	P(3)-C(61)-C(62)	122.6(5)
Rh(2)-P(2)-C(1)	117.5(3)	P(3)-C(61)-C(66)	117.3(5)
Rh(1)-P(3)-C(2)	117.9(3)	P(4)-C(71)-C(72)	118.5(6)
Rh(2)-P(4)-C(2)	113.6(3)	P(4)-C(71)-C(76)	121.4(6)
Rh(1)-P(1)-C(11)	115.5(2)	P(4)-C(81)-C(82)	120.4(5)
Rh(1)-P(1)-C(21)	115.2(2)	P(4)-C(81)-C(86)	119.6(5)
Rh(2)-P(2)-C(31)	118.9(2)	P(1)-C(1)-P(2)	111.6(4)
Rh(2)-P(2)-C(41)	108.2(2)	P(3)-C(2)-P(4)	110.5(5)

## Torsion Angles

P(1)-Rh(1)-Rh(2)-P(2)	6.31(8)	C(21)-P(1)-P(2)-C(31)	18.3(5)
P(3)-Rh(1)-Rh(2)-P(4)	7.60(9)	C(51)-P(3)-P(4)-C(81)	20.5(6)
P(1)-Rh(1)-Rh(2)-P(4)	177.36(9)	C(61)-P(3)-P(4)-C(71)	17.1(4)
P(3)-Rh(1)-Rh(2)-P(2)	163.45(8)	C(11)-P(1)-Rh(1)-Cl(1)	60.1(3)
C(1)-P(1)-P(3)-C(2)	16.2(5)	C(21)-P(1)-Rh(2)-Cl(2)	60.9(3)
C(1)-P(2)-P(4)-C(2)	15.3(5)	C(31)-P(2)-Rh(2)-Cl(2)	44.8(3)
C(11)-P(1)-P(3)-C(61)	18.2(4)	C(41)-P(2)-Rh(2)-Cl(2)	77.3(3)
C(21)-P(1)-P(3)-C(51)	17.9(4)	C(51)-P(3)-Rh(1)-Cl(1)	43.2(3)
C(31)-P(2)-P(4)-C(81)	17.4(4)	C(61)-P(3)-Rh(1)-Cl(1)	78.5(3)
C(41)-P(2)-P(4)-C(71)	17.2(4)	C(71)-P(4)-Rh(2)-Cl(2)	60.0(3)
C(11)-P(1)-P(2)-C(41)	12.2(3)	C(81)-P(4)-Rh(2)-Cl(2)	61.6(3)

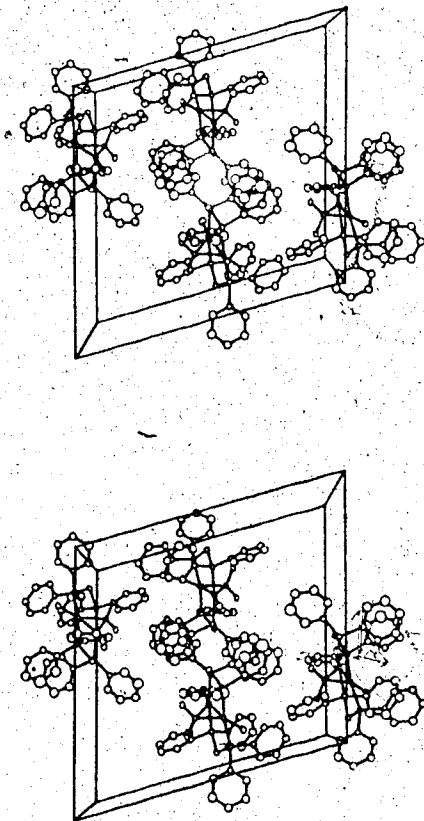


Figure 12. Cell Packing Diagram of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]_2$ .

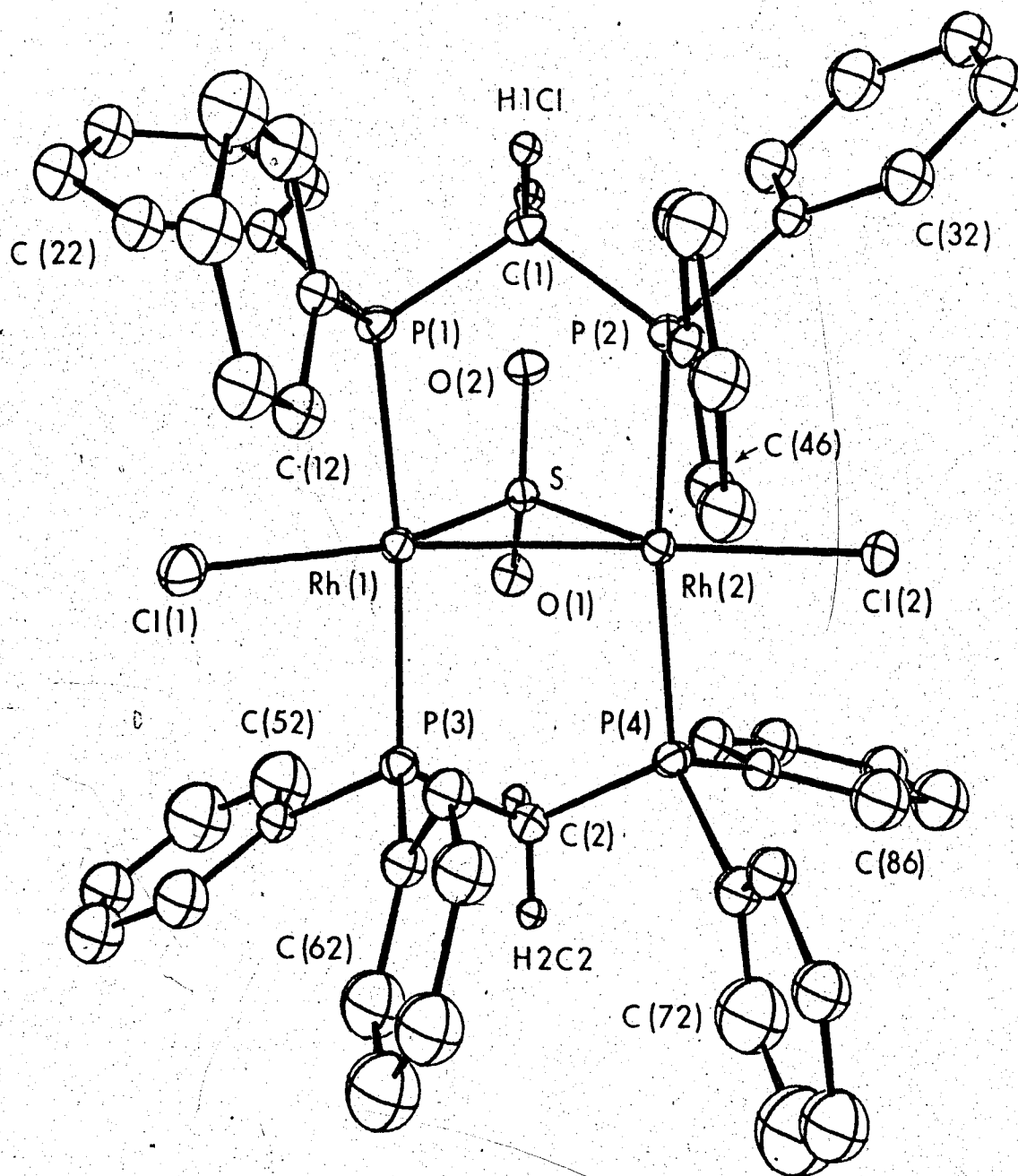


Figure 13. A Perspective View of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$ .

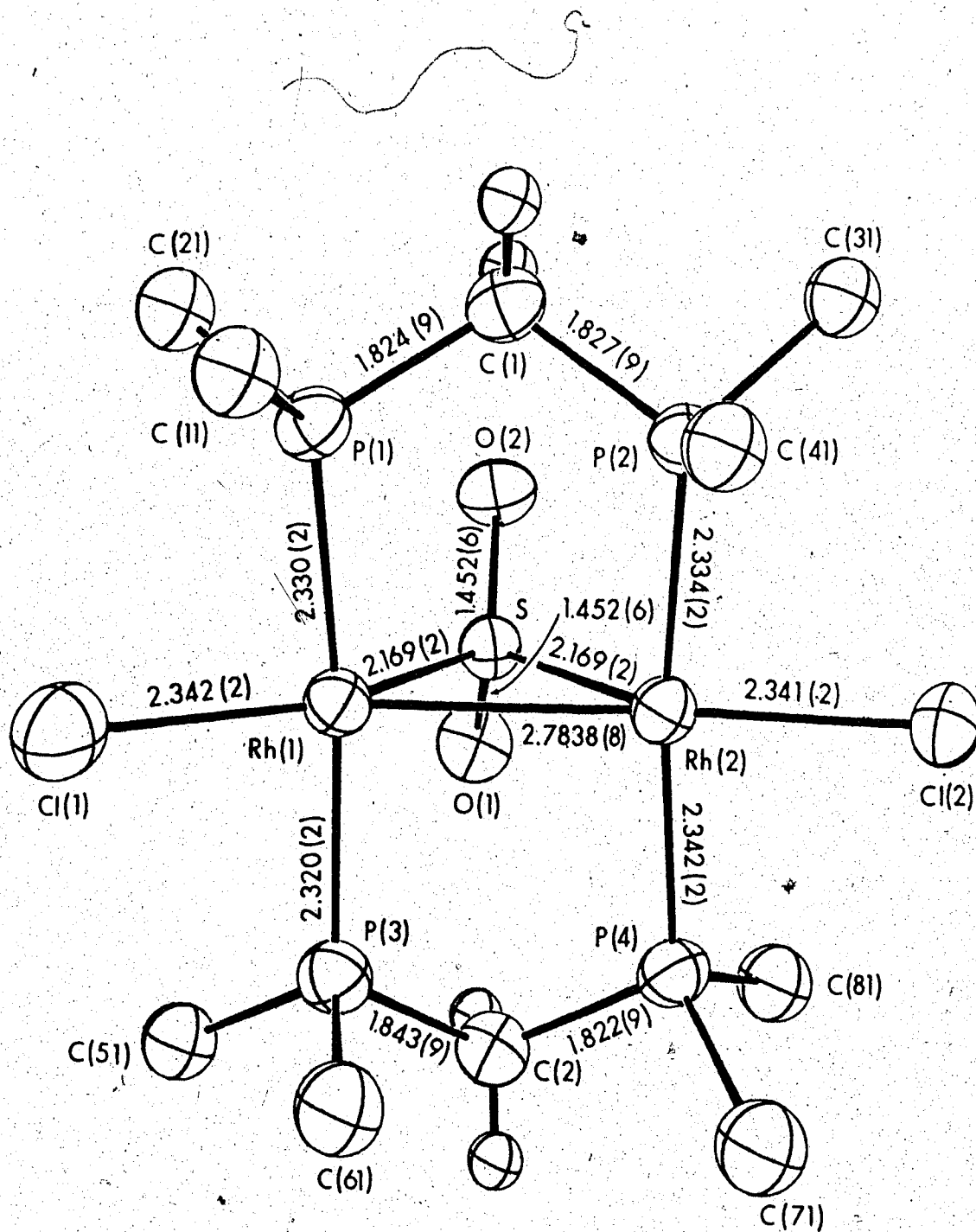


Figure 14. The Inner Coordination Sphere of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$ .

## DISCUSSION

### Description of Structure

The complex,  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$ , displays a distorted "A-frame" geometry, similar to that displayed by the palladium analogue  $[\text{Pd}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$ <sup>85</sup> (apart from the metal-metal bond in the present species). The "A" configuration is described by the chloro and sulfur dioxide ligands in the equatorial plane, with the apical position occupied by the bridging  $\text{SO}_2$  ligand. Both rhodium centres are bridged by two DPM ligands, which are mutually trans and approximately perpendicular to the equatorial plane. The distortion from the idealized "A-frame" structure which would have the terminal Cl ligands trans to the bridging  $\text{SO}_2$  ligand results both from close nonbonded contacts between the chloro ligands and the phenyl rings and from the presence of the Rh-Rh bond (see Figure 13 and Table 24). Therefore, unlike other "A-frame" complexes which have approximately square planar coordination at the metals, the present complex exhibits a highly distorted trigonal-bipyramidal metal environment with the average S-Rh-Rh, S-Rh-Cl and Cl-Rh-Rh angles (50.07(6), 142.9(5) and 166.7(5)°, respectively, see Table 25) deviating significantly from the idealized 120° value.

The Rh-Rh distance of 2.7838(9)Å is consistent with a normal Rh-Rh single bond, falling within the range previously reported for such distances (2.617(3)-2.8415(7)Å).<sup>35, 126-133</sup>

The present value can be compared to that observed in the related Rh-Rh bonded tricarbonyl species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})-(\mu\text{-Cl})(\text{DPM})_2]^+$  (2.8415(7)Å)<sup>35</sup> and can be contrasted to the distances of 3.1520(8) and 3.155(4)Å, respectively, for  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$ <sup>120</sup> and  $[\text{Rh}_2(\text{CO})_2(\mu\text{-S})(\text{DPM})_2]$ ,<sup>89</sup> in which no Rh-Rh bond is present.

The geometry of the bridging SO<sub>2</sub> ligand is consistent with a Rh-Rh bonded system. Thus the acute Rh-S-Rh angle of 79.84(7)° indicates compression along the Rh-Rh axis and is comparable to other such values obtained when SO<sub>2</sub> bridges a metal-metal bond (72.6(1) - 75.6(2)°)<sup>60,134-136</sup> but is significantly smaller than the range in M-S-M angles observed (91.2(2) - 118.0(2)°)<sup>64,85,137</sup> when SO<sub>2</sub> bridges two metal atoms which are not bonded to each other. The bonding in this SO<sub>2</sub> ligand is symmetrical (Rh(1)-S = Rh(2) - S = 2.169(2)Å) and these Rh-S distances are significantly shorter than the metal-sulfur distances observed in other sulfur dioxide bridged complexes of the second and third row platinum metals ( $[\text{Pd}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$ , Pd-S = 2.234(3) and 2.240(3)Å;<sup>85</sup>  $[\text{IrH}(\text{CO})_2(\text{PPh}_3)_2]\text{SO}_2$ , Ir-S = 2.313 Å;<sup>60</sup>  $[\text{Pd}_3(\text{SO}_2)_2(t\text{-BuNC})_5]$ , Pd-S (av.) = 2.261(9)Å;<sup>138</sup> and  $[\text{Pt}_3(\text{SO}_2)_3(\text{PPh}_3)_3]$ , Pt-S(av.) = 2.275(5)Å).<sup>136</sup> The S-O distances of 1.452(6) Å and the O-S-O angle of 111.9(4)° compare well with other determinations in which SO<sub>2</sub> acts as either a bridging or a terminal ligand<sup>52,134-138</sup> and can be compared to the analogous parameters in free SO<sub>2</sub>

(1.431(1) Å and 119.0(5)°, respectively).<sup>139</sup> The differences between free and coordinated SO<sub>2</sub> can be attributed to back donation into SO<sub>2</sub> orbitals which are slightly bonding with respect to the O-O interaction and antibonding with respect to the S-O interactions.<sup>52</sup> However, more simply they reflect the change from sp<sup>2</sup> to sp<sup>3</sup> hybridization about the sulfur atom. The Rh-S-O angles are also close to the expected tetrahedral values.

The Rh-Cl distances of 2.342(2) and 2.341(2) Å are not unusual; however they are somewhat shorter than those typically observed (range 2.355(2) - 2.386(3) Å)<sup>31,122,123,140</sup> for rhodium (I) phosphine complexes.

Within the Rh-DPM framework most parameters are usual. The Rh-P distances (average 2.331(9) Å)<sup>124</sup> are within the range normally observed when phosphine ligands are mutually trans,<sup>35,85,89,117,120</sup> and the P-C distances (both methylene and phenyl) compare well with other determinations.<sup>35,85,89,120</sup> The methylene carbon atoms of the bridging DPM ligand are folded in a cis configuration towards the sulfur dioxide ligand (see Table 23 and Figure 13). This orientation of the methylene groups allows the phenyl groups to stagger themselves with respect to the terminal chloro ligands in the equatorial plane (see Cl-Rh-P phenyl torsion angles, Table 25) and also places four of the eight phenyl rings in the open positions around the bridging site. Viewed down the Rh-Rh axis the Rh-P vectors are slightly staggered with



respect to one another as can be seen from the P-Rh-Rh-P torsion angles of  $6.31(8)^\circ$  and  $7.60(9)^\circ$ . This observed twist in the Rh-DPM framework thrusts rings 4 and 6 further into the enclosed bridging site, effectively blocking this site and resulting in short Rh-H nonbonded contacts ( $\text{Rh}(1) - \text{H}(66) = 2.70 \text{ \AA}$  and  $\text{Rh}(2) - \text{H}(46) = 2.73 \text{ \AA}$ ). Although the enclosed site is effectively blocked by these phenyl rings, the exposed terminal sites are conspicuously vacant and open to attack by small molecules.

Transformation of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\mu\text{-SO}_2)(\text{DPM})_2]^+$  to  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$

The reaction of the parent "A-frame" complex, as the  $\text{BPh}_4^-$  salt, 1a, with sulfur dioxide yields initially the sulfur dioxide adduct  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$  3a (see Figure 11). The assignment of this structure is based on (1) the infrared spectrum which is similar to that of the carbonyl adduct 2a, which has been characterized by an X-ray structural determination;<sup>35</sup> (2) the  $\text{SO}_2$  bands in the infrared spectrum at  $1230$  and  $1070 \text{ cm}^{-1}$  which are in the region observed for other  $\text{SO}_2$  ligands bridging metal-metal bonded centres;<sup>60,138</sup> (3) the  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum which displays only one phosphorus environment; (4) satisfactory elemental analysis; and (5) treatment of a solution of 3a with dinitrogen which leads to  $\text{SO}_2$  loss and isolation of the parent species 1a.

Prolonged treatment of a solution of 3a with SO<sub>2</sub> resulted in an apparent disproportionation reaction yielding [Rh<sub>2</sub>Cl<sub>2</sub>(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>] (4) as a brown microcrystalline solid and a yellow solution containing the other unidentified disproportionation product(s). Subsequent attempts to repeat the above reaction have shown that it is not a simple disproportionation reaction. When the reaction was repeated using the pure parent "A-frame", which had been recrystallized several times, it was found that the reaction stopped at the sulfur dioxide adduct 3a. Whereas when 1a was purified by only a single crystallization or if the reaction was carried out in situ without purification of 1a, the transformation of compound 3a to 4 proceeded to completion in about 4 h. This suggested the involvement of an impurity in the reaction yielding compound 4.

Since [RhHCl(DPM)<sub>2</sub>][BPh<sub>4</sub>] was known to be an impurity in some preparations of 1a,<sup>141</sup> this species was added to solutions of 3a to assess its effect on the above reaction. It was found however, that even when present in equimolar amounts this hydrido complex had no apparent effect on the reaction rate.

Another potential impurity is the [RhCl<sub>2</sub>(CO)<sub>2</sub>]<sup>-</sup> anion, which is generated as the counter ion in the initial preparation of [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-Cl)(DPM)<sub>2</sub>]<sup>+</sup> (see Chapter II). An ion exchange was then performed to replace this anion with BPh<sub>4</sub><sup>-</sup>. However, if exchange is incomplete, trace amounts

of  $[\text{Rh}(\text{Cl})_2(\text{CO})_2]^-$  may be present. To test the possible involvement of the  $[\text{RhCl}_2(\text{CO})_2]^-$  anion, we treated the complex  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{RhCl}_2(\text{CO})_2]$ , **1c**, with  $\text{SO}_2$ . Regardless of solvent, the transformation of **3** to **4** proceeded to completion in every case within 3 h. When traces of **1c** were added to pure **1a**, this reaction again occurred much more readily than with only pure **1a**, suggesting the involvement of the  $[\text{RhCl}_2(\text{CO})_2]^-$  anion as a chloride transfer agent in the reaction. It has already been shown by Balch and co-workers<sup>142</sup> that the dimer  $[\text{RhCl}(\text{CO})_2]_2$  abstracts chloride anion from *trans*- $[\text{RhCl}(\text{CO})(\text{DAM})]_2$  to give  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DAM})_2]^+$  and  $[\text{RhCl}_2(\text{CO})_2]^-$ . It is not unreasonable to expect therefore that a similar process is occurring in the transformation of **3** to **4**. In fact a model of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{RhCl}_2(\text{CO})_2]$ , constructed from data made available to us by Professor Balch,<sup>142,143</sup> shows that the anion approaches the tricarbonyl cationic species (which we assume is structurally similar to complex **3a**), in such an orientation that chloride transfer from the anion to the cation is very feasible. We believe that the species resulting from  $\text{Cl}^-$  transfer by  $[\text{RhCl}_2(\text{CO})_2]^-$ , i.e.,  $[\text{RhCl}(\text{CO})_2]$  or the dimer  $[\text{RhCl}(\text{CO})_2]_2$ , then abstracts a chloride ion from another cationic species **3a** to restart the process, resulting in a net chloride transfer reaction. The rhodium-DPM species produced is presumably a neutral dichlorodicarbonyl, sulfur

dioxide bridged species,  $[\text{Rh}_2\text{Cl}_2(\text{CO})_2(\mu\text{-SO}_2)(\text{DPM})_2]$ , which then loses CO to yield complex 4.

It is not surprising that the relatively small species  $[\text{RhCl}_2(\text{CO})_2]^-$  is accomplishing the chloride transfer as opposed to any species containing the bulky DPM ligand. Of course when the chloride ion is added directly to a solution of 3a, evaporation of this solution under a  $\text{SO}_2$  atmosphere results in quantitative conversion of 3a to 4. Therefore the conversion of complex 3a into 4 occurs in the presence of any chloride ion source. It is also of interest at this stage to note the differences between  $\text{SO}_2$  and CO in these systems. In the presence of a chloride ion source the  $\text{SO}_2$  adduct 3a is unstable, yielding complex 4, whereas the analogous tricarbonyl species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{X}]$ ,  $\text{X} = \text{Cl}^-$  (vide infra) or  $[\text{RhCl}_2(\text{CO})_2]^-$ ,<sup>142</sup> are stable and readily isolated. Two possible reasons are suggested for this difference. The bridging  $\text{SO}_2$ , we believe withdraws more electron density from the metals than the bridging CO ligands. This favours nucleophilic  $\text{Cl}^-$  attack on the  $\text{SO}_2$  adduct. Another significant difference lies in the orientation of the methylene carbon atoms of the DPM ligands. Structural studies have shown that the methylene groups fold towards the more bulky bridging equatorial group. In the carbonyl adduct this is the Cl ligand, whereas in the  $\text{SO}_2$  adduct the bulkier group is the  $\text{SO}_2$  ligand. Thus, methylene orientation in the  $\text{SO}_2$  adduct may

lead to a more favourable orientation of the phenyl rings allowing easier access of the chloride donor to the metal center.

Efforts at characterizing the other so-called disproportionation products have met with little success. On the basis of  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra of the products in this reaction, we find, in addition to resonances due to 4, that at least three other unidentified resonances occur. The sum of their integrated intensities is approximately equal to that of complex 4. It seems therefore that the second product in the reaction, species 5, is unstable and is reacting further to yield the species observed in the NMR experiment. This is consistent with the fact that the relative intensities of the bands in the infrared spectra of the yellow product changed from sample to sample. However, it was noted that no carbonyl species was ever observed in the infrared spectra of the final yellow product.

#### Reaction of $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$ with CO

Reaction of 4 with CO, was initially believed to yield the tricarbonyl species *cis*- $[\text{Rh}_2\text{Cl}_2(\text{CO})_2(\mu\text{-CO})(\text{DPM})_2]$ .<sup>96a</sup> However further investigations have shown that this tricarbonyl species is actually  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2]\text{-}[\text{Cl}]$ , 2b, (see Figure 15). It is a 1:1 electrolyte in acetone and dichloromethane solutions, its  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum is identical to that of the  $\text{BPh}_4^-$  salt, whose structure has been determined,<sup>35</sup> and its infrared spectrum is

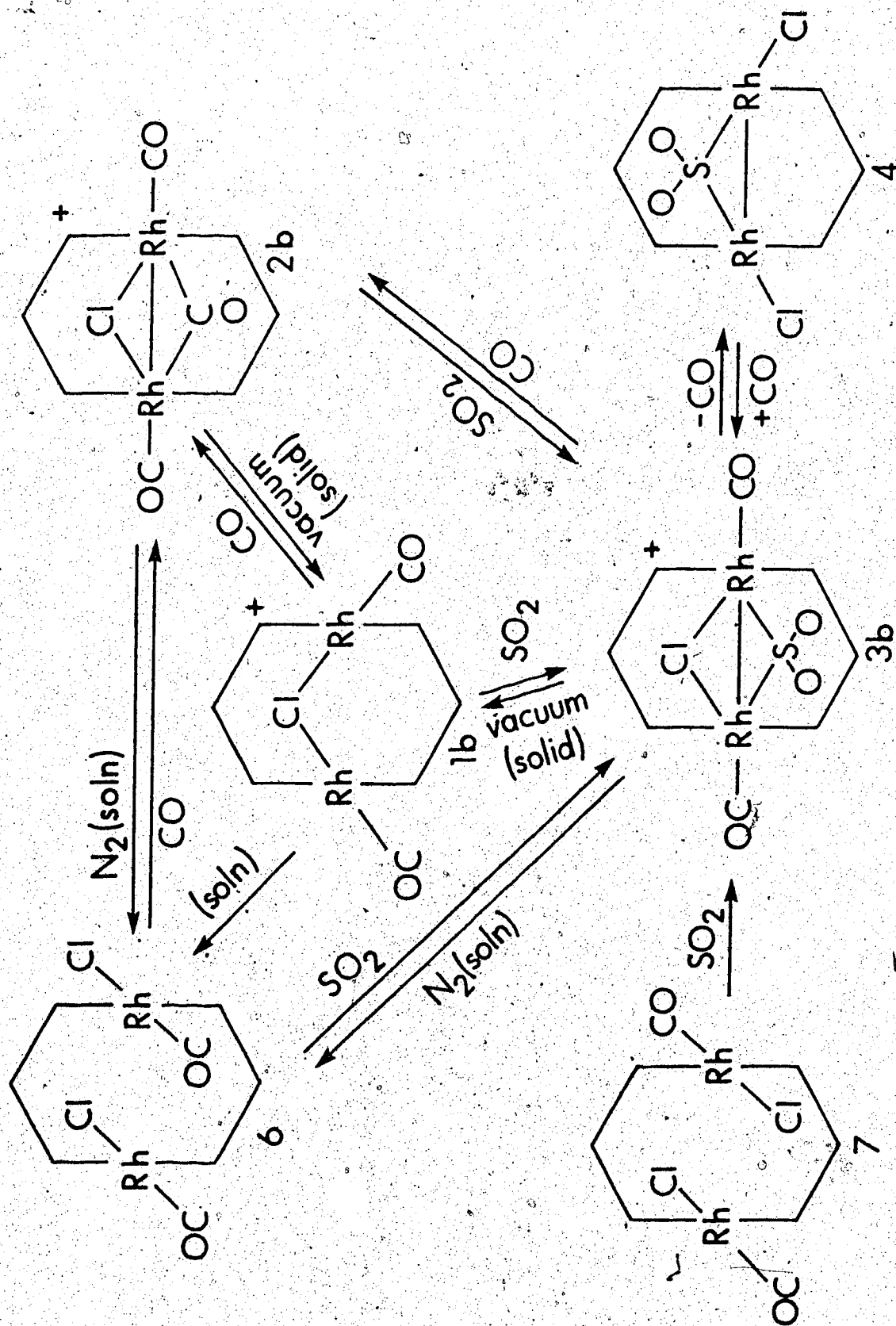


Figure 15. A Reaction Scheme for Binuclear Rh-DPM Complexes with CO and SO<sub>2</sub>.

also similar to that of the  $\text{BPh}_4^-$  salt. Under vacuum, a solid sample of 2b loses the bridging carbonyl ligand as indicated by its infrared spectrum, which is essentially identical with that of 1a (see Table 18). This species can therefore be formulated as  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2][\text{Cl}]$  (1b). A solution of 1b, however is a nonelectrolyte, and it is believed that recoordination of the chloride ion occurs such that the species present in solution is actually *cis*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  (6, see Figure 15). Complex 6 can also be obtained directly by bubbling  $\text{N}_2$  through a solution of 2b. The infrared spectra of 6 and 1b are markedly different and furthermore the  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of 6 is not similar to that of the  $\text{BPh}_4^-$  "A-frame" complex 1a. This together with the conductivity differences between 1a and 6 supports our assignment of this species as *cis*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$ . In addition, the infrared spectrum and elemental analysis of 6 are essentially identical with those of the trans analogue 7. Our formulation of 6 as the *cis* species instead of the trans isomer is based on chemical differences. Complex 6 is soluble in  $\text{CH}_2\text{Cl}_2$  and acetone whereas the trans analogue 7 is extremely insoluble. Furthermore, 6 reacts readily and reversibly with CO in  $\text{CH}_2\text{Cl}_2$  to give 2b, whereas 7 does not react even after extended periods of time. However, unambiguous assignment of complex 6 as the *cis* species must await a structural determination. The *trans*-DAM analogue, *trans*- $[\text{RhCl}(\text{CO})(\text{DAM})]_2$ , has been observed to crystallize in different

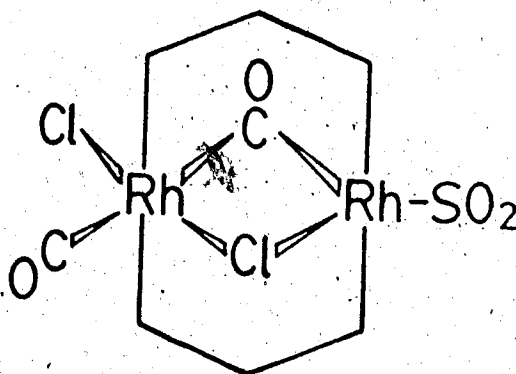
forms, <sup>31,125</sup> therefore 6 may be another crystalline modification of 7.

Both the cis and trans species (6 and 7, respectively) react with SO<sub>2</sub> to yield the species [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-Cl)(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>][Cl], 3b, which is assigned this structure on the basis of its conductivity (1:1 electrolyte) and its <sup>31</sup>P{<sup>1</sup>H} NMR spectrum which shows only one phosphorus environment and which is identical with that of its BPh<sub>4</sub><sup>-</sup> analogue 3a (vide supra). In addition, when solutions of 6 and 7 are treated for prolonged periods of time with SO<sub>2</sub>, complex 4 is obtained (see Figure 15).

Reaction of trans-[RhCl(CO)(DPM)]<sub>2</sub> with SO<sub>2</sub>

The reaction of the trans species (7) with SO<sub>2</sub> has been studied by monitoring, using infrared spectroscopy, the slow stepwise addition of SO<sub>2</sub>. Initially species are observed which contain bridging carbonyl ligands ( $\nu_{\text{CO}} = 1740 \text{ cm}^{-1}$ ). Upon completion of the reaction none of these species is observed; instead only the symmetric SO<sub>2</sub>-bridged species 3b remains. In addition a solution containing the initially formed product of the SO<sub>2</sub> reaction with 7 is nonconducting for several minutes (although on the basis of spectral and colour changes it is obvious that a reaction has occurred) after which it becomes a 1:1 electrolyte. The above data are consistent with terminal attack of SO<sub>2</sub> and formation of an intermediate species of the form:





This species is then believed to lose  $\text{Cl}^-$  and to rearrange to the final product 3b, having a bridging  $\text{SO}_2$  ligand. The possibility that the carbonyl vibration at  $1740\text{ cm}^{-1}$  is due to the monocarbonyl species  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  (see Chapter V), which was observed in the analogous reaction with  $\text{CS}_2$  at intermediate times, is ruled out since this species is never detected in the  $^{31}\text{P}$  NMR spectra of this reaction.

Site of  $\text{SO}_2$  attack in  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$

In these "A-frame" species, there are two potential sites of attack, either directly at the enclosed site, bridging the metal centres, or at a terminal, exposed position remote from the bridging site. It has been shown that CO attacks la terminally, forcing one of the previously coordinated ligands into the bridging site.<sup>35,91</sup> Likewise CO appears to attack the  $\text{SO}_2$  "A-frame" complex 4 terminally since no evidence is obtained for attack at

the bridging site. In contrast,  $\text{SO}_2$  appears to attack complex 1 directly at the bridging site, which has been shown by the structural determination of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})\text{-}(\text{DPM})_2][\text{BF}_4]$  to be open<sup>120</sup> (see Chapter II). Spectroscopic evidence supports  $\text{SO}_2$  attack at the bridging site. The infrared spectra obtained during the slow stepwise addition of  $\text{SO}_2$  to 1a displayed no bands assignable to bridging carbonyl species. On the basis of the analogous reaction of 1 with CO and of the reaction of the *trans*-dichloro-dicarbonyl species 7 with  $\text{SO}_2$  (vide supra), both of which occur by terminal attack, we would have anticipated observing species with bridging CO bands in the infrared spectra, if attack of  $\text{SO}_2$  on 1 were also terminal. Furthermore even at  $-50^\circ\text{C}$  when the reaction is monitored by  $^{31}\text{P}\{^1\text{H}\}$  NMR techniques the only resonances observed are assignable to the symmetric species 1a and 3a. If attack were terminal, it is anticipated that resonances assignable to an asymmetrical species would be observed. We believe therefore that, on the basis of the above data, terminal attack of 1 with  $\text{SO}_2$  can be ruled out, since no asymmetric species were detected. Furthermore we feel that it is unlikely that a facile rearrangement is operating since no simple rearrangement mechanism can be devised that would readily yield the symmetric bridged species 3a from terminal attack. The reasons for the varying modes of CO and  $\text{SO}_2$  in complex 1 is at the present time not obvious, although

attack by the better  $\pi$ -acid ( $\text{SO}_2$ ) would be favoured at the bridging site since in this site both electron rich metals can donate electron density to this ligand.

## CHAPTER V.

### Unusual Structural and Chemical Trends Within a Series of Binuclear Rhodium Carbonyl Halide Complexes

#### INTRODUCTION

The reaction of  $\text{SO}_2$  with *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  (1) and *trans*- $[\text{RhCl}(\text{CO})(\text{DAM})]_2$  (2) is believed to proceed through an intermediate of the form  $[\text{Rh}_2\text{Cl}(\text{CO})(\text{SO}_2)(\mu\text{-Cl})(\mu\text{-CO})(\text{L-L})_2]$  (L-L = DPM or DAM)<sup>96</sup> (Chapter IV). However, this intermediate is short lived in the case of DPM and is not observed in the case of DAM, making definitive characterization impossible. Since the stabilities of these intermediates appear to change on going from DPM to DAM as the bridging ligand, it was felt that by changing halides, it might have been possible to isolate this intermediate, as a result of the increased steric bulk of the bromo and iodo ligands slowing the rearrangement process. Therefore the preparation of the previously unreported *trans*-dibromo and *trans*-diiodo, DPM complexes and the *trans*-diiodo, DAM complex was attempted.

#### EXPERIMENTAL

Preparation of  $[\text{Rh}_2\text{I}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{I}]$ ,  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  and  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$

Typically 0.100 g of *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$ <sup>66</sup> was suspended in 15 mL of  $\text{CH}_2\text{Cl}_2$  and to this a five fold excess of

the halide salt (NaBr, KI), in a minimum volume of methanol, was added. After ca. 12 h the solution was concentrated to about 15 mL then precipitated with diethyl ether and dried in vacuum, yielding  $[\text{Rh}_2\text{X}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{X}]$  (X = Br, I). However in solution the bromo species undergoes CO loss at room temperature over a period of 24 h, or on refluxing in  $\text{CH}_2\text{Cl}_2$  for 2 h yielding  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ . The analogous chloro complex,  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  was obtained as a red-brown species in solution on refluxing a toluene suspension of *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  for 12 h. Recrystallization of all species was from methylene chloride and diethyl ether. Typical yields were from 70 to 90%. Elemental analyses:  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ :  $\text{C}_{51}\text{H}_{44}\text{Br}_2\text{O}_1\text{P}_4\text{Rh}_2$ ; calc. C, 52.70; H, 3.81; Br, 13.7; Found C, 52.3; H, 3.70; Br, 13.0;  $[\text{Rh}_2\text{I}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{I}]$ :  $\text{C}_{52}\text{H}_{44}\text{I}_2\text{O}_2\text{P}_4\text{Rh}_2$ ; calc. C, 48.62; H, 3.45; Found C, 48.25; H, 3.51. See Table 26 for spectral data.

### Reactions with $\text{SO}_2$ and $\text{CO}$

#### (a) Dicarboxyl Species

Typically 0.100 g of  $[\text{RhX}(\text{CO})(\text{DPM})]_2$  or  $[\text{RhX}(\text{CO})(\text{DAM})]_2$  (X = Cl, Br, I) in 15 mL of  $\text{CH}_2\text{Cl}_2$  was treated with  $\text{SO}_2$  or  $\text{CO}$  for 10 min, the volume was reduced under a stream of the reactant gas to about 7 mL and then the products were precipitated with diethyl ether saturated with the reactant

Table 26. Spectral Data for the Complexes

No.	Complex	Infrared Absorption Maxima (cm <sup>-1</sup> ) <sup>a</sup>	<sup>31</sup> P{ <sup>1</sup> H}nmr Chemical Shifts (ppm) <sup>b</sup>
3	[Rh <sub>2</sub> Br(μ-CO)(CO)(DPM) <sub>2</sub> ][Br]	1958(s), 1800(m)	25.0 (multiplet)
4a	[Rh <sub>2</sub> Cl <sub>2</sub> (μ-CO)(DPM) <sub>2</sub> ]	1745(σ)	19.7 (115.9 Hz)
4b	[Rh <sub>2</sub> Br <sub>2</sub> (μ-CO)(DPM) <sub>2</sub> ]	1745(s)	19.4 (114.7 Hz)
5	[Rh <sub>2</sub> I(μ-CO)(CO)(DPM) <sub>2</sub> ][I]	1955(s), 1810(m)	21.5 (multiplet)
6,7	[Rh <sub>2</sub> I <sub>2</sub> (CO) <sub>2</sub> (DAM) <sub>2</sub> ]	1965(sh), 1940(s), 1820(m)	-
9a	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-CO)(μ-Cl)(DPM) <sub>2</sub> ][Cl]	2004(m), 1960(s), 1868(m)	29.8 (94.0)
9b	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-CO)(μ-Br)(DPM) <sub>2</sub> ][Br]	2005(m), 1968(s), 1865(m)	28.7 (93.8)
9c	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-CO)(μ-I)(DPM) <sub>2</sub> ][I]	1990(sh), 1970(s), 1860(m)	26.6 (92.7)
10a	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-SO <sub>2</sub> )(μ-Cl)(DPM) <sub>2</sub> ][Cl]	2010(s), 1980(sh) 1230(m), 1070(m)	24.5 (91.6)
10b	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-SO <sub>2</sub> )(μ-Br)(DPM) <sub>2</sub> ][Br]	2005(s), 1970(sh) 1230(m), 1085(m)	27.0 (90.6)
10c	[Rh <sub>2</sub> (μ-SO <sub>2</sub> )(μ-I)(CO) <sub>2</sub> (DPM) <sub>2</sub> ][I]	2005(m), 1990(s) 1210(m), 1065(m)	26.0 (90.3)
11	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-CO)(μ-I)(DAM) <sub>2</sub> ][I]	2005(m), 1958(s), 1860(m)	-
12	[Rh <sub>2</sub> (CO) <sub>2</sub> (μ-SO <sub>2</sub> )(μ-I)(DAM) <sub>2</sub> ][I]	1985(s), 1205(m), 1065(m)	-
13a	[Rh <sub>2</sub> Cl <sub>2</sub> (μ-SO <sub>2</sub> )(DPM) <sub>2</sub> ]	1191(m), 1063(s)	19.6 (113.5)
13b	[Rh <sub>2</sub> Br <sub>2</sub> (μ-SO <sub>2</sub> )(DPM) <sub>2</sub> ]	1190(m), 1060(s)	21.1 (113.6)

<sup>a</sup>Infrared spectra were run as nujol mulls on KBr plates; s, strong; m, medium; w, weak; sh, shoulder.

<sup>b</sup><sup>31</sup>P{<sup>1</sup>H}nmr chemical shifts are relative to H<sub>3</sub>PO<sub>4</sub> (downfield positive), coupling constants (|<sup>1</sup>J<sub>Rh-P</sub> + <sup>x</sup>J<sub>Rh-P</sub>|) are given in parentheses. The solvent used was CD<sub>2</sub>Cl<sub>2</sub>.

gas. Yields of the expected products,  $[\text{Rh}_2(\text{CO})_2(\mu\text{-L})(\mu\text{-X})(\text{DPM})_2][\text{X}]$  ( $\text{L} = \text{CO}, \text{SO}_2$ ;  $\text{X} = \text{Cl}, \text{Br}, \text{I}$ ) averaged *ca.* 75%. The reversibility of the CO and  $\text{SO}_2$  reactions were studied by dissolving the products of these reactions in  $\text{CH}_2\text{Cl}_2$  and bubbling  $\text{N}_2$  through the solution for up to 48 h.

#### (b) Monocarbonyl Species

Typically 200 mg of sample was dissolved in 2 mL of  $\text{CD}_2\text{Cl}_2$  and the reactant gas introduced a bubble at a time. The  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra were recorded, at  $-50^\circ\text{C}$ . After each addition of gas until no significant changes were observed. The infrared spectra were recorded in an analogous manner using 200 mg of sample in 20 mL of  $\text{CH}_2\text{Cl}_2$ .

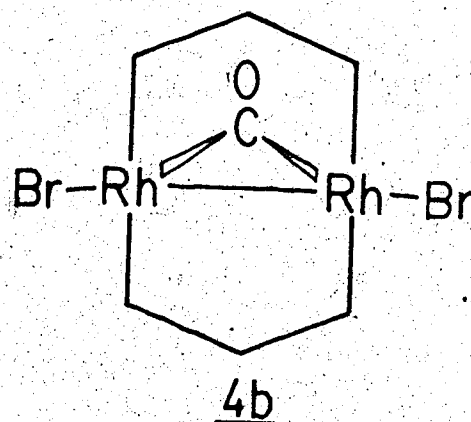
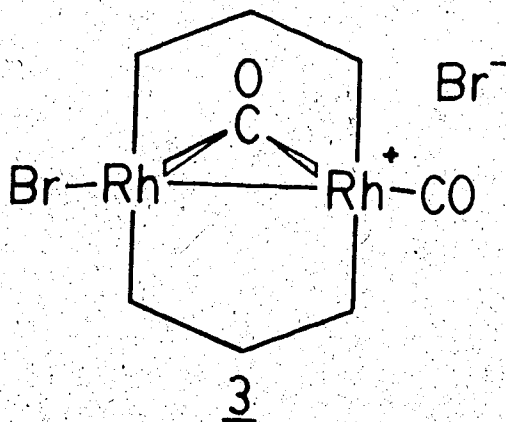
### DISCUSSION

#### Halide Exchange Reactions

The products of the halide exchange reactions show interesting chemical and structural trends which seem to depend on the steric bulk of the halide ligands and also on the crowding at the two metal centres as governed by the bridging DPM and DAM groups.

The reaction of *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  (1), with NaBr yields initially  $[\text{Rh}_2\text{Br}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{Br}]$  (3), a species with bands in the infrared spectrum at 1958 and  $1800\text{ cm}^{-1}$ , consistent with terminal and bridging carbonyl ligands. This species is a 1:1 electrolyte in acetone ( $70\text{ ohm}^{-1}\text{ cm}^{-2}\text{ mole}^{-1}$ ) and its  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum, which is similar to the iodo species,

shown in Figure 16, (vide infra) indicates an asymmetric structure. This evidence coupled with elemental analysis leads to the formulation of 3 as shown below



In solution complex 3 recoordinates  $\text{Br}^-$  and undergoes CO loss, over a period of several hours, to yield  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  (4b), which has been characterized by an X-ray structure determination<sup>144</sup> (see Chapter VI). The  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of this species is shown in Figure 16 and is consistent with the symmetric structure observed in the solid state. All  $^{31}\text{P}\{^1\text{H}\}$  NMR parameters (Table 26) are in excellent agreement with those of the analogous species  $[\text{Rh}_2\text{X}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  ( $\text{X} = \text{Cl}, \text{Br}$ ).<sup>96</sup> A solution of 4b is non conducting. The analogous chloro complex,  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  (4a) is obtained on refluxing a suspension of the *trans*-dichloro dicarbonyl species 1. This reaction has also been observed by Professor Balch and coworkers,<sup>143</sup> although it is not clear whether the species isolated by



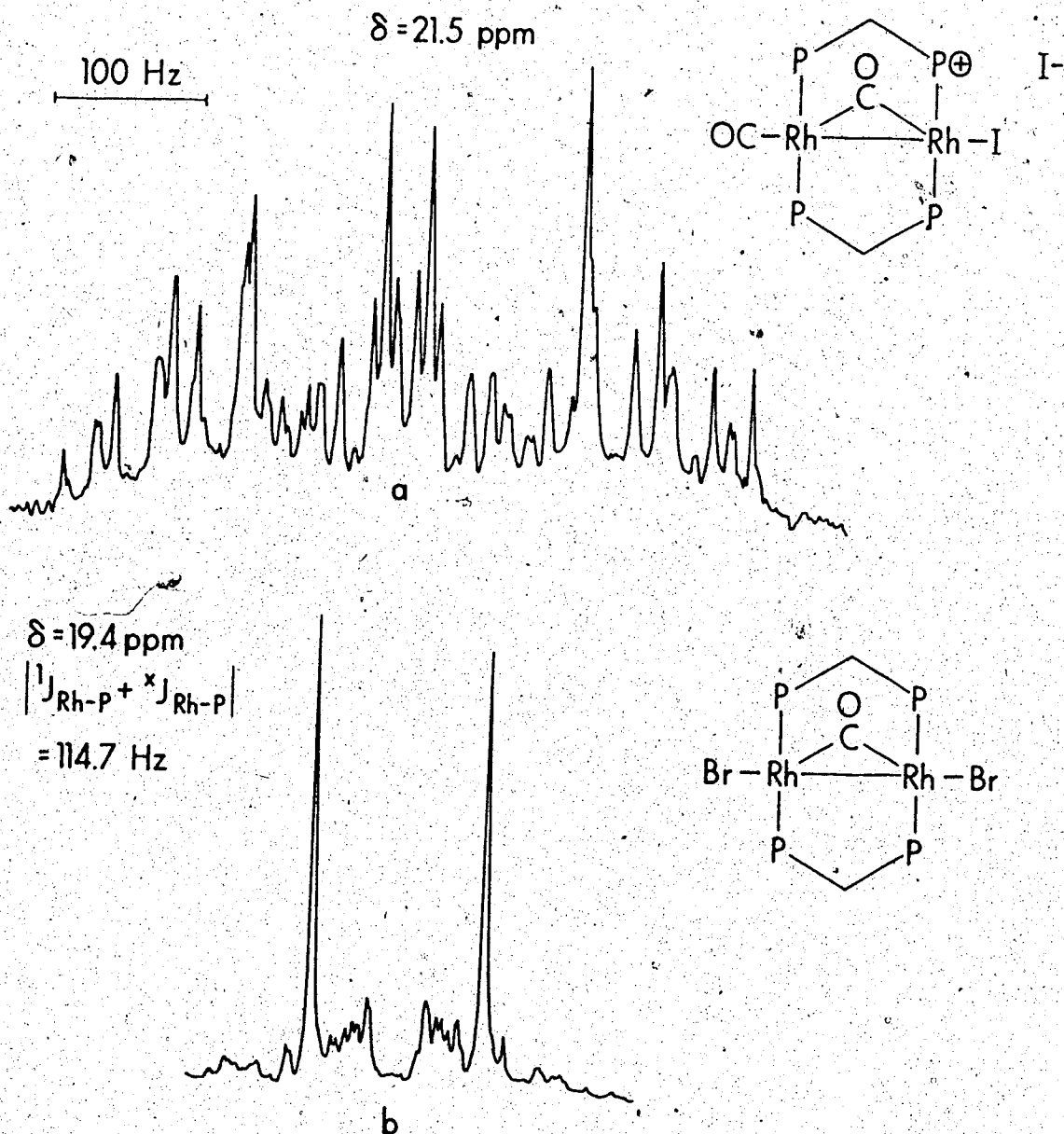


Figure 16. The  $^{31}\text{P}\{^1\text{H}\}$  NMR Spectra at 223 K of a)  $[\text{Rh}_2\text{I}(\text{CO})-(\mu\text{-CO})(\text{DPM})_2][\text{I}]$  and b)  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ .

these workers is identical to the one which we observe.

The reaction of 1 with KI yields  $[\text{Rh}_2\text{I}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{I}]$  (5), analogous to complex 3. The carbonyl bands in the infrared spectrum are observed at 1955 and 1810  $\text{cm}^{-1}$  and the  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum (Figure 16) is consistent with the asymmetric structure proposed. Complex 5 is a 1:1 electrolyte in solution. Unlike complex 3 however, complex 5 is stable under  $\text{N}_2$  in solution and does not undergo CO loss.

The bromo DAM species, *trans*- $[\text{RhBr}(\text{CO})(\text{DAM})]_2$ , is known and is probably structurally similar to *trans*-dichloro-dicarbonyl DAM species (2).<sup>66</sup> Iodide exchange on complex 2 yields a species which infrared studies and elemental analysis indicate is probably a mixture of the *trans*-diiodo-dicarbonyl complex, *trans*- $[\text{RhI}(\text{CO})(\text{DAM})]_2$  (6) and an asymmetric species  $[\text{Rh}(\text{CO})(\mu\text{-CO})(\text{DAM})_2][\text{I}]$  (7), which is probably similar to DPM species 5. The asymmetric species comprises 75% of the product.

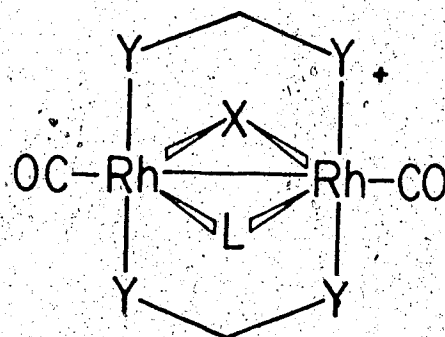
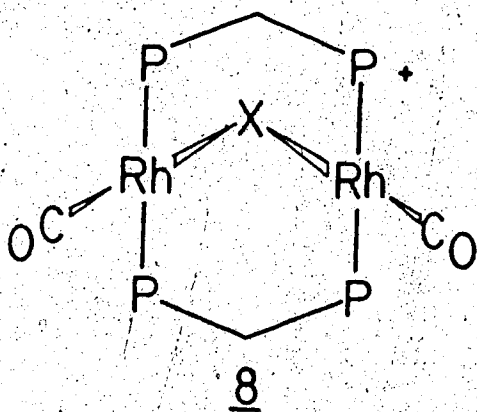
The structural trends observed in the above series of DPM and DAM halides is therefore consistent with steric bulk arguments indicating that the *trans* configuration of equatorial ligands, as observed in the dichloro species 1 and 2, and in *trans*- $[\text{RhBr}(\text{CO})(\text{DAM})]_2$ , is destabilized with bulkier halide ligands. The larger steric bulk of the bromo ligand, compared to the chloro ligand, does not favour simultaneous coordination of both bromo and both carbonyl ligands in the DPM complex and the asymmetric, ionic species

is formed initially. When bromide recoordination does occur, it is accompanied by CO loss to give the monocarbonyl species 4b. With the DPM ligand, the stable iodo species is the asymmetric complex 5, again because simultaneous coordination of all iodo and carbonyl ligands is not favoured due to steric crowding. Furthermore, the large size of  $I^-$  does not favour its recoordination and CO loss is not observed in this species. The effect of the large DAM ligand is seen in the dibromo DAM species which still exists as the trans complex  $[RhBr(CO)(DAM)]_2$ , unlike its DPM analogue. The DAM ligand presumably allows more room to accommodate the larger bromo ligand. Even with the bulkier iodo ligand some *trans*- $[RhI(CO)(DAM)]_2$  6 is observed together with the asymmetric species 7.

### Reactions with CO

#### i) Dicarbonyl Species

It is interesting that no evidence is seen for the symmetric "A-frame" species 8 ( $X = Br, I$ ), even though the reaction of 3 and 5 with CO and  $SO_2$  yield species 9 and 10, respectively, which are analogous to the products obtained (9a and 10a) by the reaction of 8a ( $X = Cl$ ) with these small molecules.<sup>35,91,96</sup> The  $^{31}P\{^1H\}$  NMR spectra of the tricarbonyl species 9b and 9c ( $X = Br, I$ , respectively,  $L = CO$ ) show one phosphine environment and are extremely similar to that of the chloro analogue,  $[Rh_2(CO)_2(\mu-CO)(\mu-Cl)(DPM)_2]^+$  9a, whose structure has been determined.<sup>35,142</sup> These DPM



9 L=CO, Y=P

10 L=SO<sub>2</sub>, Y=P

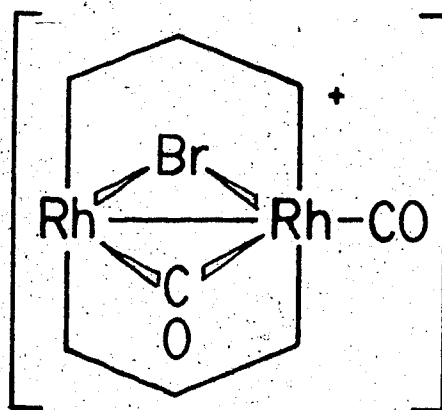
11 L=CO, Y=As, X=I

12 L=SO<sub>2</sub>, Y=As, X=I

tricarbonyl complexes show an interesting trend in  $^{31}\text{P}$  shifts and coupling constants (Cl, Br, I;  $\delta = 29.6, 28.7, 26.6$  ppm;  $|\ ^1J_{\text{Rh-P}} + \ ^xJ_{\text{Rh-P}} | = 94.2, 93.8, 92.7$  Hz, respectively). Furthermore, the infrared data for compounds 9a, 9b and 9c are all closely comparable. The complexes, *trans*-[RhX(CO)<sub>3</sub>(DAM)]<sub>2</sub> (X=Cl, Br), like their DPM chloro analogue, 1 show no reaction with CO under our conditions. Reaction of the mixture of iodo-DAM species 6 and 7 with CO however results in the isolation of a tricarbonyl species 11, which appears from its infrared spectrum, to be analogous to 9b and 9c.

An investigation of the ease of decarbonylation of complexes 9 shows a notable trend. The chloro complex 9a readily loses CO in solution under an N<sub>2</sub> stream or in the solid state under vacuum,<sup>35,91</sup> the bromo species 9b on the

other hand does not lose CO in the solid state under vacuum even after 72 h but loses it slowly in solution to give complex 3 and subsequently complex 4b. The iodo species 9c does not lose CO in either the solid state or in solution. The DAM-iodo species 11 undergoes CO loss slowly in solution under an N<sub>2</sub> stream. On decarbonylation of the bromo tricarbonyl species 9b, the complex initially produced is the asymmetric species 3. This is consistent with the findings of Mague and coworkers<sup>35,91</sup> which indicate that in the chlorotricarbonyl complex 9a, it is initially a terminal carbonyl group which is lost with the bridging carbonyl ligand then moving to the terminal site. Assuming the same mechanism for the bromo analogue, the intermediate species after carbonyl loss would then be:



Because of the large size of the bromo ligand it is this ligand which moves to the less sterically encumbered terminal site yielding species 3, whereas in the chloro

species migration of the carbonyl ligand is favoured, presumably for electronic reasons.

ii) Monocarbonyl Species

Reaction of  $[\text{Rh}_2\text{X}_2(\mu\text{-CO})(\text{DPM})_2]$  ( $\text{X} = \text{Cl}$ , 4a;  $\text{X} = \text{Br}$ , 4b) with excess CO results in the formation of the tricarbonyl species 9a and 9b. When slow stepwise reaction of 4b with CO is monitored by  $^{31}\text{P}\{^1\text{H}\}$  NMR spectroscopy, resonances are observed which are assignable to the asymmetric dicarbonyl species 3 and to the tricarbonyl complex 9b. Complex 3 is observed throughout the reaction but only in trace amounts. In contrast, the monocarbonyl species is found in significant quantities until completion of the reaction. It seems therefore that CO reacts preferentially with 3 compared to 4b.

If instead of reacting 4a with excess CO, the CO is added slowly, *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})_2]$  (1) precipitates from solution (see Figure 17). The observation of two products (1 and 9a) from slow and rapid addition, respectively, of CO suggests the presence of an intermediate dicarbonyl species,  $[\text{Rh}_2\text{Cl}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{Cl}]$  3a, analogous to the bromo species 3. We postulate that on slow CO addition attack of this intermediate by  $\text{Cl}^-$  occurs giving complex 1, whereas in the presence of excess CO (ie. during rapid CO addition), attack by CO predominates yielding instead the tricarbonyl species 9a. Based on our other work with related "A-frame" species<sup>96b,144</sup> and on a consideration of

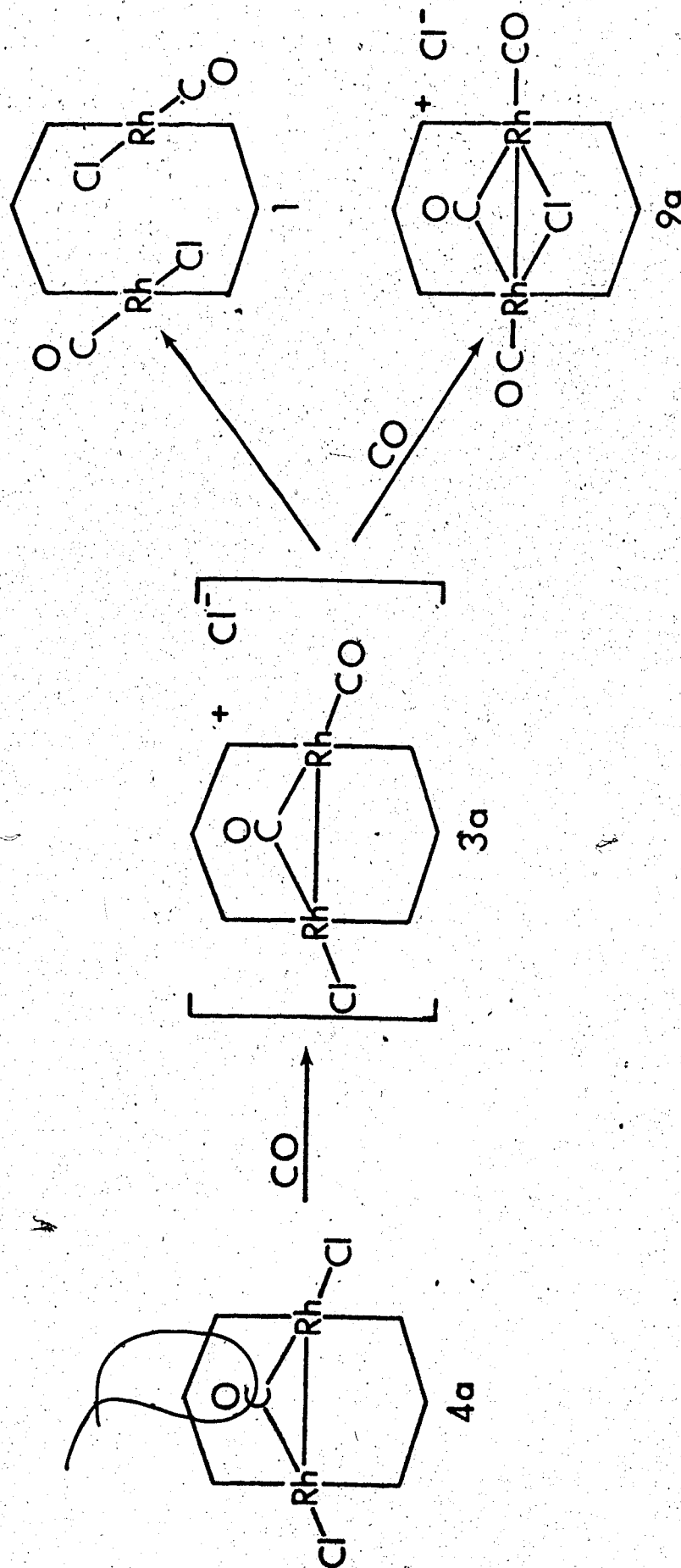
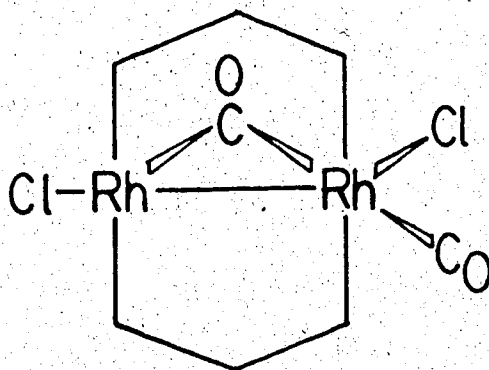


Figure 17. A Scheme for the Reaction of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  with CO.

the electronic preference of each metal we would predict that  $\text{Cl}^-$  attack on species 3a (Figure 17) occurs at the metal site between the bridging and terminal CO ligands yielding a species as shown below, which could then rearrange to the *trans*-dichlorodicarbonyl species (1).



Support of this postulated intermediate comes from the structural determination<sup>145</sup> of an analogous species which has  $(\text{MeO})_2\text{PN}(\text{Et})\text{P}(\text{OMe})_2$  instead of the DPM ligands and adopts this asymmetric geometry. Similarly if CO attacks species 3a between the bridging carbonyl and chloro ligand, as we believe it does, complex 9a is obtained by a facile shift of the chloro ligand into the bridging position.

#### Reactions with $\text{SO}_2$

##### i) Dicarboxyl Species

The  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra of  $\text{SO}_2$  adducts 10b and 10c are consistent with one phosphine environment in each case and are similar to that obtained for  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-Cl})-$



$(\text{DPM})_2]^+ 10a^{96}$  (see Chapter IV) (Cl, Br, I;  $\delta = 24.6, 27.0, 26.0$ ;  $|^1J_{\text{Rh-P}} + ^xJ_{\text{Rh-P}}| = 91.6, 90.6, 90.3$  Hz, respectively). In addition the infrared spectra of 10b and 10c are comparable to that of 10a leading to the formulation of these species as shown previously. Preliminary studies with *trans*- $[\text{RhX}(\text{CO})(\text{DAM})]_2$  (X = Cl, Br), indicate that these complexes react in a manner similar to *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  yielding initially  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-X})(\text{DAM})_2][\text{X}]$  and eventually undergoing CO loss yielding  $[\text{Rh}_2\text{X}_2(\mu\text{-SO}_2)(\text{DAM})_2]$ . Similarly the iodo complexes 6 and 7 react with  $\text{SO}_2$  to yield an  $\text{SO}_2$  adduct  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-I})(\text{DAM})_2][\text{I}]$  12 analogous to the DPM complexes.

The bromo species,  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-Br})(\text{DPM})_2][\text{Br}]$  (10b), on prolonged  $\text{SO}_2$  treatment, undergoes a decarbonylation reaction yielding  $[\text{Rh}_2\text{Br}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  13b, paralleling the chemistry of the chloro analogue.<sup>96b</sup> In contrast, the iodo species 10c does not undergo this reaction. Studies on the conversion of  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-Cl})(\text{DPM})_2]$  to  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  indicated that chloride ion coordination was required before CO loss was observed (Chapter IV), so we assume that although  $\text{Br}^-$  coordination occurs in 10b the increased steric bulk of the iodo ligand prevents coordination of a second  $\text{I}^-$  ion in 10c and therefore prevents CO loss.

Although  $\text{SO}_2$  can be readily removed from species 10a it is not removed from complexes 10b and 10c. The bromo

species 10b instead undergoes CO loss in solution under an N<sub>2</sub> flush to yield 13b, whereas 10c loses neither CO nor SO<sub>2</sub>.

ii) Monocarbonyl Species

The reaction of  $[\text{Rh}_2\text{X}_2(\mu\text{-CO})(\text{DPM})_2]$  (X = Cl, 4a; X = Br, 4b) with SO<sub>2</sub> yields as the final products  $[\text{Rh}_2\text{X}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  (13a and 13b) and  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-X})(\text{DPM})_2][\text{X}]$  (10a and 10b) for the chloro and bromo complexes, respectively. When these reactions are monitored, during the slow stepwise addition of SO<sub>2</sub>, utilizing <sup>31</sup>P{<sup>1</sup>H} NMR spectroscopy, several unexpected products are observed. The spectra of the reaction of 4b with SO<sub>2</sub> show the presence of two asymmetric species (3 and 14b) and four symmetric species (4b, 9b, 10b and 13b) at different times during the experiment (see Figure 18). Of these species only 14b has not been previously characterized by us. This species we tentatively assign as a monocarbonylmonosulfur dioxide species, possibly having the structure shown. This asymmetric structure is consistent with the <sup>31</sup>P{<sup>1</sup>H} NMR pattern observed and the infrared data which show an SO<sub>2</sub> species with a terminal carbonyl ligand as one of the first products. Of course, 14b is not an unreasonable initial product in the reaction. All other species can be explained by facile CO transfer from this species to others present in solution. Although Figure 18 is not meant to represent unambiguously the sequence of events, it does present some plausible steps in the production of the ob-

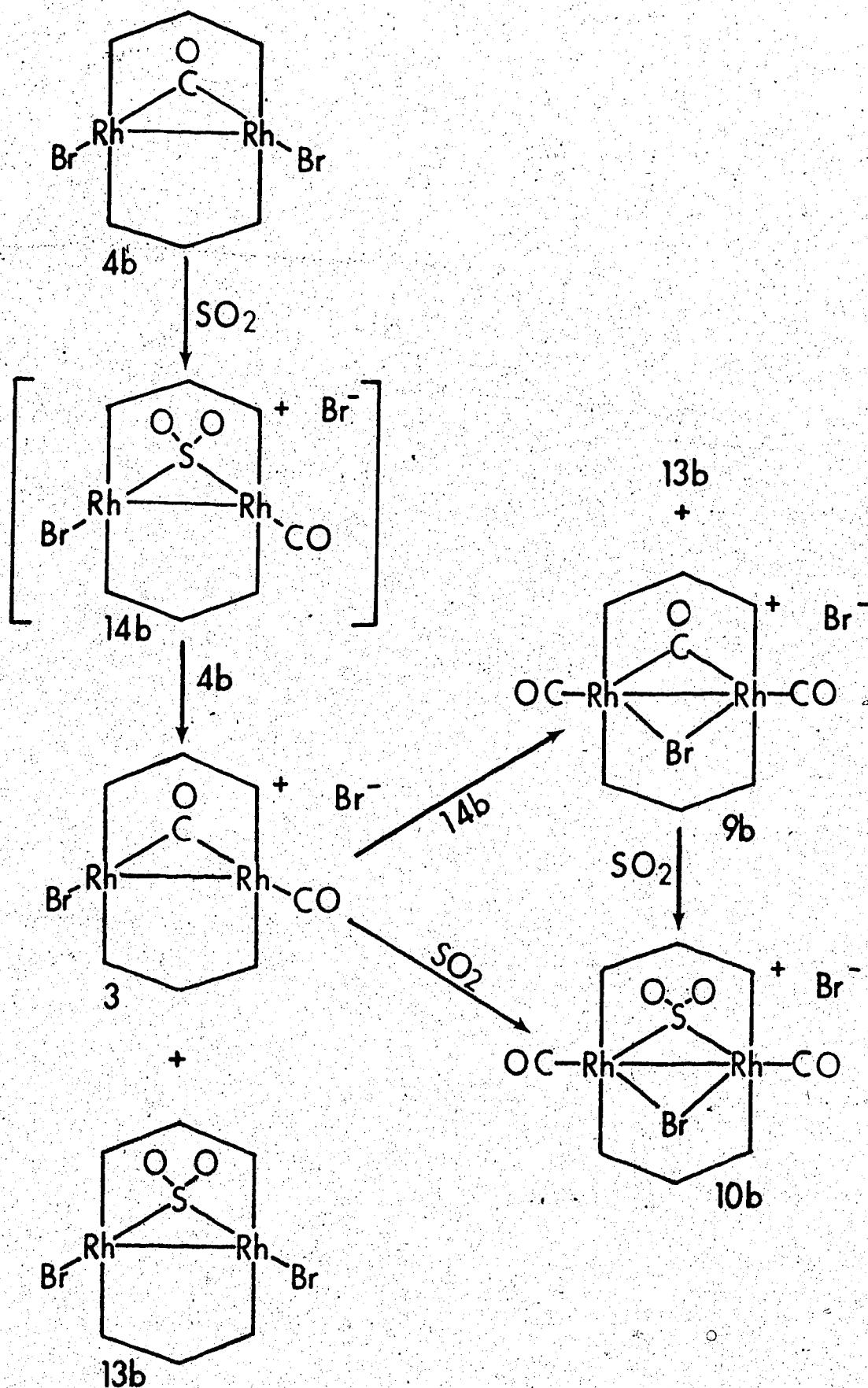


Figure 18. A Possible Reaction Sequence for the Reaction of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  with  $\text{SO}_2$ .

served species, and in particular offers some rationale for the production of di- and tricarbonyl products from a monocarbonyl reactant. For example, CO transfer from 14b to 4b would yield 3 and one of the final products, 13b. The other final product in the reaction, 10b, can be obtained by the reaction of 3 with SO<sub>2</sub>. Complex 3 can also react with 14b yielding more of 13b and the tricarbonyl species 9b which can subsequently react with SO<sub>2</sub> giving 10b.

The analogous reaction of 4a with SO<sub>2</sub> seems to proceed by a simpler route. Again an asymmetric species 14a tentatively assigned as being analogous to the bromo species 14b, is observed in the NMR experiment. However only two other species 10a and 13a are observed, resulting from CO transfer from one molecule of 14a to another. There may be other intermediates in this reaction but none is observed.

### Summary

We have seen in these halide complexes an interesting structural trend which is dependent on halide size and on the relative dimensions of the DPM and DAM ligands. The chemistries of these halide species with CO and SO<sub>2</sub> also show interesting trends which again can be attributed, at least in part, to steric interaction between the ligands. Also notable in this chemistry is the strong tendency toward symmetric species. Only in the two iodo species 5 and 7, where steric bulk of the iodo ligand inhibits the chemistry favoured by the other halide species, are the asym-

metric species stable. Therefore the asymmetric complex  $[\text{Rh}_2\text{Br}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{Br}]$  either loses CO yielding the symmetric species  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  or gains CO to give another symmetric species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Br})(\text{DPM})_2][\text{Br}]$ . This tendency toward symmetric species is commonly observed throughout our binuclear chemistry with the DPM and DAM ligands (Chapter IV) but is in contrast to analogous complexes with the related methoxydiphenylazane ligand,  $(\text{MeO})_2\text{PN}(\text{Et})\text{P}(\text{OMe})_2$ , which show a tendency toward asymmetric species.<sup>145</sup>

## CHAPTER VI.

### The Structure of $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ : A Binuclear Rhodium Carbonyl Complex Having an Unusually Low Carbonyl Stretching Frequency

#### INTRODUCTION

The reaction of *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  with NaBr initially yields an asymmetric species  $[\text{Rh}_2\text{Br}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{Br}]$  which undergoes a rearrangement in solution to give a symmetric species having an unusually low value for  $\nu(\text{CO})$  of  $1745 \text{ cm}^{-1}$  (see Chapter V).<sup>126</sup> Based on spectral data, elemental analyses, and its chemistry with  $\text{SO}_2$  this symmetric product can be equally well formulated as  $[\text{RhBr}(\mu\text{-CO})(\text{DPM})]_2$ , containing two "ketonic" carbonyl ligands, or as  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ , having one carbonyl ligand and a formal Rh-Rh bond. The low value of the carbonyl vibration is consistent with a "ketonic" carbonyl formulation, being comparable to the value observed in  $[\text{Pd}_2\text{Cl}_2(\mu\text{-CO})(\text{DAM})_2]$ <sup>32</sup> and  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\mu\text{-DMA})(\text{DPM})_2]$ <sup>42</sup> which contain "ketonic" carbonyl ligands and the  $^{31}\text{P}\{^1\text{H}\}$  NMR is very similar to other symmetric dirhodium species which have no metal-metal bond.<sup>120,146,147</sup> Furthermore, its reaction with  $\text{SO}_2$  yields the dicarbonyl species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-SO}_2)(\mu\text{-Br})(\text{DPM})_2][\text{Br}]$  as one of the final products. However, this data can also be interpreted in terms of a monocarbonyl formulation. The analogous  $\text{SO}_2$ -bridged compound<sup>96</sup>

$[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  (Chapter IV), has a low value for  $\nu(\text{SO})$  and has  $^{31}\text{P}\{^1\text{H}\}$  NMR parameters very similar to those in the present carbonyl compound, although it has a formal Rh-Rh bond. In addition, the formation of a dicarbonyl product in the reaction with  $\text{SO}_2$  can be explained by CO transfer from one molecule to another (see Chapter V) since a carbonyl-free species,  $[\text{Rh}_2\text{Br}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  is also observed.

The structure determination was therefore undertaken in order to unambiguously establish the mode of carbonyl bonding.

### EXPERIMENTAL

#### Crystallization of $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$

A (50 mg) sample of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})_x(\text{DPM})_2]$  ( $x = 1, 2$ ), prepared as described in Chapter V, was dissolved in 3 mL of  $\text{CH}_2\text{Cl}_2$  from which well formed crystals were obtained by slow diethyl ether diffusion. The crystals were analyzed spectrally as either  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  or  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})_2(\text{DPM})_2]$ .

#### Data Collection

A clear red plate of the title complex was mounted on a glass fibre. Preliminary film data showed that the crystal belonged to the monoclinic system with extinctions ( $h0l, h+l\text{ odd}; 0k0, k\text{ odd}$ ) characteristic of the centrosymmetric space group  $P2_1/n$ , a non standard setting of  $P2_1/c$ .

Data collection was as previously described in Chapter II and pertinent crystal and intensity collection data are presented in Table 27.

### Structure Solution and Refinement

The positions of the Rh, Br and P atoms were obtained by direct methods using MULTAN.<sup>148</sup> The remaining atoms were located from subsequent least-squares refinements and electron density difference maps. Anomalous dispersion terms for Rh, Br and P<sup>108</sup> were included in  $F_c$ . All carbon atoms of the phenyl rings were refined as rigid groups having  $D_6h$  symmetry and C-C distance of 1.392 Å. The hydrogen atoms were included as fixed contributions and were not refined. All non group atoms were refined individually with anisotropic thermal parameters (see Chapter II for a more detailed discussion).

The final model with 205 parameters varied converged to  $R = 0.045$  and  $R_w = 0.055$ .<sup>121</sup> In the final electron density difference map the highest 20 peaks were in the vicinities of either the phenyl groups or the Rh and Br atoms (0.45 - 0.25  $e/\text{Å}^3$ ). A typical carbon atom on earlier syntheses had an electron density of about 3.5  $e/\text{Å}^3$ .

### Results

The positional and thermal parameters for the individual anisotropic atoms, rigid group atoms and idealized hydrogen parameters are given in Tables 28, 29 and 30 respectively. Least-squares plane calculations are pre-



Table 27. Summary of Crystal Data and Intensity Collection  
for  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$

Compound	$[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$																																												
Formula	$\text{C}_{51}\text{H}_{44}\text{Br}_2\text{O}_1\text{P}_4\text{Rh}_2$																																												
Formula Weight	1162.4 amu																																												
Cell Parameters																																													
a	20.429 (2) Å																																												
b	11.895 (1) Å																																												
c	18.865 (2) Å																																												
$\beta$	100.275 (9)°																																												
V	4510.7 Å <sup>3</sup>																																												
Z	4																																												
Density	1.711 (calc'd.)																																												
Space Group	$\text{C}_{2h}^5\text{-P2}_1/\text{n}$ (non-standard setting of $\text{P2}_1/\text{c}$ )																																												
Crystal Dimensions	0.240 x 0.088 x 0.301 mm																																												
Crystal Volume	0.00442 mm <sup>3</sup>																																												
Crystal Faces (and distances from an arbitrary origin within the crystal (mm))	<table border="0"> <tbody> <tr><td>0</td><td>1</td><td>0</td><td>(0.044)</td></tr> <tr><td>0</td><td><math>\bar{1}</math></td><td>0</td><td>(0.044)</td></tr> <tr><td>1</td><td>0</td><td>0</td><td>(0.138)</td></tr> <tr><td><math>\bar{1}</math></td><td>0</td><td>0</td><td>(0.098)</td></tr> <tr><td>0</td><td>0</td><td><math>\bar{1}</math></td><td>(0.156)</td></tr> <tr><td><math>\bar{1}</math></td><td>0</td><td>2</td><td>(0.131)</td></tr> <tr><td><math>\bar{2}</math></td><td>0</td><td><math>\bar{1}</math></td><td>(0.120)</td></tr> <tr><td><math>\bar{2}</math></td><td><math>\bar{1}</math></td><td><math>\bar{1}</math></td><td>(0.094)</td></tr> <tr><td>1</td><td>1</td><td>0</td><td>(0.082)</td></tr> <tr><td>1</td><td><math>\bar{1}</math></td><td>0</td><td>(0.059)</td></tr> <tr><td>1</td><td>0</td><td>1</td><td>(1.103)</td></tr> </tbody> </table>	0	1	0	(0.044)	0	$\bar{1}$	0	(0.044)	1	0	0	(0.138)	$\bar{1}$	0	0	(0.098)	0	0	$\bar{1}$	(0.156)	$\bar{1}$	0	2	(0.131)	$\bar{2}$	0	$\bar{1}$	(0.120)	$\bar{2}$	$\bar{1}$	$\bar{1}$	(0.094)	1	1	0	(0.082)	1	$\bar{1}$	0	(0.059)	1	0	1	(1.103)
0	1	0	(0.044)																																										
0	$\bar{1}$	0	(0.044)																																										
1	0	0	(0.138)																																										
$\bar{1}$	0	0	(0.098)																																										
0	0	$\bar{1}$	(0.156)																																										
$\bar{1}$	0	2	(0.131)																																										
$\bar{2}$	0	$\bar{1}$	(0.120)																																										
$\bar{2}$	$\bar{1}$	$\bar{1}$	(0.094)																																										
1	1	0	(0.082)																																										
1	$\bar{1}$	0	(0.059)																																										
1	0	1	(1.103)																																										
Temperature	20°C																																												
Radiation	$\text{CuK}\alpha$ ( $\lambda=1.540562$ Å) filtered with 0.5 mil thick nickel foil)																																												
$\mu$	98.229 cm <sup>-1</sup>																																												
Range in Absorption Correction Factors	0.190 - 0.476																																												
Receiving Aperture	6x6 mm, 30 cm from the crystal																																												

Table 27, continued

Takeoff Angle	3.9°
Scan Speed	2° in 20/min
Scan Range	1.00° below $K\alpha_1$ to 1.00° above $K\alpha_2$
Background Counting Time	10s ( $3^\circ < 2\theta < 45^\circ$ ) 20s ( $45^\circ < 2\theta < 96^\circ$ ) 40s ( $96^\circ < 2\theta < 120^\circ$ )
$2\theta$ limits	$3^\circ < 2\theta < 120^\circ$
$2\theta$ units for centred reflections	$(60^\circ < 2\theta < 70^\circ)$
Final number of variables	205
Unique Data Collected	7071
Unique Data Used ( $F_o^2 \geq 3\sigma(F_o^2)$ )	4718
Error in observation of unit weight	1.392
R	0.045
$R_w$	0.055

sented in Table 31 and selected bond length and angles are shown in Tables 32 and 33, respectively. A listing of observed and calculated structure amplitudes is available.<sup>110</sup>

A stereoview of the unit cell of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  is shown in Figure 19. The crystallographic  $a$  axis is horizontal to the right, the  $c$  axis runs from the bottom to the top and the  $b$  axis goes into the page. Figure 20 presents a perspective view of the compound including the numbering scheme, 50% thermal ellipsoids are drawn. The inner coordination sphere is shown in Figure 21 along with some relevant bond lengths, 50% thermal ellipsoids are drawn.

TABLE 28. Positional and Thermal Parameters For The Nonhydrogen Atoms of [Rh<sub>2</sub>Br<sub>2</sub>(μ-CO)(DPM)<sub>2</sub>].

Atom	x <sup>a</sup>	y	z	U <sub>11</sub> <sup>b</sup>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Rh(1)	0.58004(3)	0.093336(5)	0.32748(3)	2.10(3)	2.26(3)	2.89(3)	0.06(2)	0.98(2)	-0.06(3)
Rh(2)	0.44867(3)	0.15824(5)	0.31124(3)	1.99(3)	2.13(3)	3.44(4)	-0.01(2)	0.61(2)	0.25(3)
Br(1)	0.69272(4)	0.03208(8)	0.31204(6)	3.03(4)	3.94(5)	5.79(6)	0.57(4)	1.96(4)	-0.37(5)
Br(2)	0.33105(5)	0.20589(9)	0.26417(8)	2.60(5)	3.90(5)	13.0(1)	0.10(4)	-0.32(5)	1.93(7)
P(1)	0.61619(9)	0.2724(2)	0.3085(1)	2.35(9)	2.56(9)	2.7(1)	-0.21(8)	1.02(8)	-0.01(8)
P(2)	0.47370(9)	0.3473(2)	0.3022(1)	2.36(9)	2.32(9)	3.2(1)	0.10(8)	0.67(8)	-0.06(9)
P(3)	0.55003(9)	-0.0946(2)	0.3208(1)	2.5(1)	2.31(9)	3.8(1)	0.14(8)	1.02(8)	0.15(9)
P(4)	0.40793(9)	-0.0248(2)	0.3104(1)	2.31(9)	2.37(9)	3.3(1)	-0.26(8)	0.57(8)	0.45(9)
O	0.5269(3)	0.1498(6)	0.4559(3)	4.0(3)	6.5(4)	2.7(4)	0.9(3)	1.3(3)	-0.9(3)
C(1)	0.5210(4)	0.1375(6)	0.3938(5)	2.5(4)	2.2(4)	4.6(6)	-0.5(3)	1.3(4)	-0.3(4)
C(2)	0.5613(4)	0.3818(6)	0.3346(4)	2.4(4)	2.7(4)	3.0(5)	-0.2(3)	0.5(3)	-0.6(3)
C(3)	0.4716(4)	-0.1243(6)	0.3513(4)	3.0(4)	2.5(4)	3.1(5)	0.4(3)	1.2(3)	0.3(3)

<sup>a</sup> Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

<sup>b</sup> The form of the thermal ellipsoid is:  $\exp[-2\pi i(x'U_{11}h'+b'U_{22}k'+c'U_{33}l'+2a'b'U_{12}hk'+2a'c'U_{13}hl'+2b'c'U_{23}kl')]$ . The quantities given in the table are the thermal coefficients  $\times 10^3$ .

TABLE 29. Derived Parameters For the Rigid Group Atoms of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{OPM})_2]$ .

Atom	X	Y	Z	B(A <sup>2</sup> )	Atom	X	Y	Z	B(A <sup>2</sup> )
C(11)	0.6232(3)	0.3053(5)	0.2153(2)	2.5(1)	C(51)	0.6042(3)	-0.2070(4)	0.3643(5)	3.1(2)
C(12)	0.6298(3)	0.4160(4)	0.1937(3)	3.8(2)	C(52)	0.5958(5)	-0.2493(5)	0.4308(3)	3.8(2)
C(13)	0.6387(3)	0.4391(4)	0.1238(3)	4.3(2)	C(53)	0.6360(5)	-0.3367(5)	0.4626(4)	5.2(2)
C(14)	0.6412(3)	0.3515(5)	0.0754(2)	4.6(2)	C(54)	0.6846(3)	-0.3817(4)	0.4278(5)	5.0(2)
C(15)	0.6347(3)	0.2407(4)	0.0970(3)	4.8(2)	C(55)	0.6931(5)	-0.3393(5)	0.3612(3)	5.4(3)
C(16)	0.6257(3)	0.176(4)	0.1670(3)	3.5(2)	C(56)	0.6529(5)	-0.2520(5)	0.3295(4)	4.3(2)
C(21)	0.6969(3)	0.3113(5)	0.3614(3)	2.3(1)	C(61)	0.5346(3)	-0.1274(6)	0.2240(3)	3.0(2)
C(22)	0.7070(4)	0.2903(4)	0.4352(8)	3.1(2)	C(62)	0.5191(4)	-0.0366(4)	0.1774(4)	3.6(2)
C(23)	0.7674(6)	0.3183(5)	0.4783(6)	3.6(2)	C(63)	0.5057(4)	-0.0540(5)	0.1033(3)	5.1(2)
C(24)	0.8177(3)	0.3672(5)	0.4478(3)	3.4(2)	C(64)	0.5078(3)	-0.1622(6)	0.0757(3)	5.8(3)
C(25)	0.8076(4)	0.3882(4)	0.3740(8)	3.4(2)	C(65)	0.5233(4)	-0.2530(4)	0.1222(4)	6.1(3)
C(26)	0.7472(6)	0.3603(5)	0.3308(6)	2.9(2)	C(66)	0.5367(4)	-0.2356(5)	0.1963(3)	4.7(2)
C(31)	0.4569(3)	0.3856(5)	0.2071(3)	2.4(1)	C(71)	0.3700(3)	-0.0935(5)	0.2259(2)	2.4(1)
C(32)	0.4441(3)	0.4956(4)	0.1836(3)	3.5(2)	C(72)	0.3549(3)	-0.2076(5)	0.2272(3)	3.7(2)
C(33)	0.4321(3)	0.5198(4)	0.1103(3)	4.7(2)	C(73)	0.3229(3)	-0.2606(4)	0.1648(3)	4.0(2)
C(34)	0.4329(3)	0.4338(5)	0.0603(3)	5.0(2)	C(74)	0.3059(3)	-0.1997(5)	0.1011(2)	4.3(2)
C(35)	0.4458(3)	0.3238(4)	0.0838(3)	4.7(2)	C(75)	0.3211(3)	-0.0857(5)	0.0999(3)	5.0(2)
C(36)	0.4578(3)	0.2996(4)	0.1572(3)	3.7(2)	C(76)	0.3531(3)	-0.0326(4)	0.1623(3)	3.9(2)
C(41)	0.4304(3)	0.4574(4)	0.3449(3)	2.4(1)	C(81)	0.3454(4)	-0.0352(5)	0.3681(5)	2.1(1)
C(42)	0.3636(3)	0.4783(5)	0.3176(4)	3.9(2)	C(82)	0.3619(2)	0.0074(4)	0.4378(5)	3.3(2)
C(43)	0.3301(2)	0.5628(5)	0.3475(3)	4.5(2)	C(83)	0.3157(5)	0.0042(4)	0.4837(7)	4.2(2)
C(44)	0.3633(3)	0.6264(4)	0.4048(3)	4.1(2)	C(84)	0.2529(4)	-0.0415(5)	0.4601(5)	3.8(2)
C(45)	0.4301(3)	0.6054(5)	0.4321(4)	3.9(2)	C(85)	0.2363(2)	-0.0840(4)	0.3904(5)	3.8(2)
C(46)	0.4636(2)	0.5209(5)	0.4021(3)	3.3(2)	C(86)	0.2825(5)	-0.0809(4)	0.3445(7)	2.9(2)

## Rigid Group Parameters

	a	XC	YC	Zc	Delta	Epsilon	Eta
Ring1	0.6322(2)	0.3284(4)	0.3284(4)	0.1454(2)	3.201(4)	1.450(4)	2.943(3)
Ring2	0.7573(2)	0.3993(3)	0.3993(3)	0.4046(2)	4.279(4)	2.126(9)	0.605(8)
Ring3	0.4449(2)	0.4097(4)	0.4097(4)	0.1337(2)	2.992(4)	1.717(4)	2.931(3)
Ring4	0.3968(2)	0.5419(3)	0.5419(3)	0.3748(2)	-0.720(4)	2.782(5)	4.429(5)
Ring5	0.6444(2)	-0.2943(4)	-0.2943(4)	0.3960(2)	-0.728(4)	1.086(6)	1.553(5)
Ring6	0.5212(2)	-0.1448(4)	-0.1448(4)	0.1498(3)	3.023(4)	1.786(4)	3.292(4)
Ring7	0.3380(2)	-0.1466(4)	-0.1466(4)	0.1635(2)	0.224(4)	2.000(4)	2.658(3)
Ring8	0.2991(2)	-0.0383(3)	-0.0383(3)	0.4141(2)	1.119(4)	0.895(8)	6.345(8)

a XC, YC and Zc are the fractional coordinates of the centroid of the rigid group.

b The rigid group orientation angles Delta, Epsilon and Eta (radians) are the angles by which the rigid body is rotated with respect to a set of axes X, Y and Z. The origin is the centre of the ring; X is parallel to a\*, Z is parallel to c and Y is parallel to the line defined by the intersection of the plane containing a\* and b\* with the plane containing b and c.

TABLE 30. Idealized Positional and Thermal Parameters For the Hydrogen Atoms of [Rh2Br2(mu-CO)(DPM)2].

Atom	x	y	z	B(A <sup>2</sup> )	Atom	x	y	z	B(A <sup>2</sup> )
H(1C2)	0.5714	0.4512	0.3121	3.10	H(45)	0.4522	0.6483	0.4717	4.90
H(2C2)	0.5698	0.3905	0.3843	3.10	H(46)	0.5090	0.5068	0.4211	4.26
H(1C3)	0.4784	-0.1174	0.4025	3.29	H(52)	-0.5629	-0.2178	0.4549	4.92
H(2C3)	0.4580	-0.1985	0.3383	3.29	H(53)	0.6304	-0.3650	0.5082	5.97
H(12)	0.6285	0.4758	0.2267	4.57	H(54)	0.7117	-0.4416	0.4493	6.04
H(13)	0.6430	0.5146	0.1088	5.25	H(55)	0.7255	-0.3709	0.3370	6.17
H(14)	0.6469	0.3672	0.0274	5.38	H(56)	0.6580	-0.2237	0.2837	5.37
H(15)	0.6363	0.1809	0.0639	5.78	H(62)	0.5184	0.0373	0.1964	4.62
H(16)	0.6217	0.1421	0.1818	4.26	H(63)	0.4946	0.0082	0.0716	6.06
H(22)	0.6726	0.2562	0.4558	3.97	H(64)	0.4971	-0.1739	0.0250	6.74
H(23)	0.7740	0.3039	0.5286	4.46	H(65)	0.5233	-0.3269	0.1030	6.67
H(24)	0.8586	0.3866	0.4773	4.33	H(66)	0.5471	-0.2977	0.2278	5.45
H(25)	0.8418	0.4216	0.3533	4.34	H(72)	0.3668	-0.2495	0.2702	4.54
H(26)	0.7404	0.3739	0.2804	4.08	H(73)	0.3130	-0.3383	0.1650	5.14
H(32)	0.4438	0.5541	0.2176	4.17	H(74)	0.2842	-0.2351	0.0583	5.10
H(33)	0.4241	0.5947	0.0941	5.60	H(75)	0.3093	-0.0431	0.0567	5.72
H(34)	0.4256	0.4501	0.0102	5.71	H(76)	0.3631	0.0457	0.1619	4.81
H(35)	0.4469	0.2648	0.0497	5.49	H(82)	0.4046	0.0396	0.4532	4.27
H(36)	0.4685	0.2242	0.1732	4.58	H(83)	0.3271	0.0341	0.5309	5.24
H(42)	0.3413	0.4357	0.2780	4.91	H(84)	0.2215	-0.0435	0.4916	4.86
H(43)	0.2845	0.5771	0.3286	5.48	H(85)	0.1934	-0.1156	0.3746	4.70
H(44)	0.3399	0.6834	0.4255	4.95	H(86)	0.2709	-0.1101	0.2969	3.95

Table 31. Least-Squares Plane Calculations

Plane no.	Equation <sup>a</sup>
1	$0.0657X - 0.1380Y - 0.9883Z + 5.4452 = 0.0$
2	$0.1007X - 0.0040Y - 0.9941Z + 4.8736 = 0.0$
3	$0.2867X + 0.9530Y - 0.0975Z - 3.5520 = 0.0$

deviation from planes, Å

Plane no.	Rh(1)	Rh(2)	Br(1)	Br(2)	P(1)	P(2)	P(3)	P(4)	C(1)	C(2)	C(3)
1	-0.0091(6)	0.0097(6)									0
2	-0.0053(6)	0.0056(6)			0.098(2)	0.100(2)				-0.639(8) <sup>b</sup>	
3	-0.0044(5)	0.0066(5)	0.0037(9)	-0.012(1)			0.063(2)	-0.060(2)	-0.034(7)		-0.683(8) <sup>b</sup>
											-0.032(7)

<sup>a</sup>X, Y, Z are orthogonal coordinates (Å) with X along the a axis, Y in the a-b plane and Z along the c\* axis.

<sup>b</sup>Not included in least squares plane calculations.

Table 32. Selected Distances (Å) in  $[\text{Rh}_2\text{Br}_2(\text{H}_2\text{CO})(\text{DPM})_2]$ 

Rh(1)-Rh(2)	2.7566(8)		P(1)-C(2)	1.841(8)	} 1.832(8)
Rh(1)-Br(1)	2.481 (1)		P(2)-C(2)	1.832(7)	
Rh(2)-Br(2)	2.474 (1)		P(3)-C(3)	1.830(8)	
Rh(1)-C(1)	1.958 (8)		P(4)-C(3)	1.825(7)	
Rh(2)-C(1)	1.961 (8)		P(1)-C(11)	1.831(5)	} 1.833(7)
Rh(1)-P(1)	2.303 (2)	} 2.317(11) <sup>a</sup>	P(1)-C(21)	1.828(4)	
Rh(1)-P(3)	2.316 (2)		P(2)-C(31)	1.824(5)	
Rh(2)-P(2)	2.319 (2)		P(2)-C(41)	1.844(4)	
Rh(2)-P(4)	2.330 (2)		P(3)-C(51)	1.833(5)	
C(1)-O <sub>a</sub>	1.167 (9)		P(3)-C(61)	1.840(5)	
C(1)-O <sub>b</sub>	1.192 (9)		P(4)-C(71)	1.835(4)	
			P(4)-C(81)	1.826(4)	

## Nonbonded Distances

P(1)-P(2)	3.026(3)	Br(2)-H(42)	2.75
P(3)-P(4)	2.992(3)	H1C2-H(12)	2.17
Rh(1)-H(62)	2.65	H2C2-H(46)	2.06
Rh(2)-H(36)	2.81	H1C3-H(52)	2.19
C(12)-H(26)	2.59	H2C3-H(72)	2.15
C(56)-H(66)	2.68	H(33)-H(65) <sup>c</sup>	2.21
C(72)-H(86)	2.61	H(35)-H(65) <sup>d</sup>	2.25
Br(1)-H(56)	3.15		

<sup>a</sup>For averaged quantities, the estimated standard deviation is the larger of an individual standard deviation or the standard deviation of a single observation as calculated from the mean.

<sup>b</sup>Riding Motion Corrected; Atom O riding on atom C(1).

<sup>c</sup>Atom located at  $x, 1+y, z$ .

<sup>d</sup>Atom located at  $1-x, \bar{y}, \bar{z}$ .



Table 33. Selected Angles (deg) in  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ 

Rh(2)-Rh(1)-Br(1)	167.06(4)	Rh(1)-P(3)-C(51)	123.1(2)
Rh(2)-Rh(1)-P(1)	93.24(5)	Rh(1)-P(3)-C(61)	104.8(2)
Rh(2)-Rh(1)-P(3)	91.22(5)	Rh(2)-P(4)-C(71)	121.2(2)
Rh(2)-Rh(1)-C(1)	45.3 (2)	Rh(2)-P(4)-C(81)	110.3(2)
Br(1)-Rh(1)-C(1)	147.6 (2)	C(2)-P(1)-C(11)	105.2(3)
Br(1)-Rh(1)-P(1)	85.62(5)	C(2)-P(1)-C(21)	102.0(3)
Br(1)-Rh(1)-P(3)	87.25(5)	C(2)-P(2)-C(31)	105.8(3)
P(1)-Rh(1)-P(3)	166.78(8)	C(2)-P(2)-C(41)	102.2(3)
P(1)-Rh(1)-C(1)	95.9 (2)	C(3)-P(3)-C(51)	102.2(3)
P(3)-Rh(1)-C(1)	96.1 (2)	C(3)-P(3)-C(61)	105.5(3)
Rh(1)-Rh(2)-Br(2)	165.45(5)	C(3)-P(4)-C(71)	103.7(3)
Rh(1)-Rh(2)-P(2)	93.24(5)	C(3)-P(4)-C(81)	103.1(3)
Rh(1)-Rh(2)-P(4)	94.51(5)	C(11)-P(1)-C(21)	104.6(3)
Rh(1)-Rh(2)-C(1)	45.2 (2)	C(31)-P(2)-C(41)	103.4(3)
Br(2)-Rh(2)-C(1)	149.2 (2)	C(51)-P(3)-C(61)	105.8(3)
Br(2)-Rh(2)-P(2)	87.96(5)	C(71)-P(4)-C(81)	104.8(3)
Br(2)-Rh(2)-P(4)	83.61(5)	P(1)-C(11)-C(12)	120.7(3)
P(2)-Rh(2)-P(4)	171.41(7)	P(1)-C(11)-C(16)	119.2(3)
P(2)-Rh(2)-C(1)	92.0 (2)	P(1)-C(21)-C(22)	117.3(3)
P(4)-Rh(2)-C(1)	96.1 (2)	P(1)-C(21)-C(26)	122.7(3)
Rh(1)-C(1)-Rh(2)	89.4 (4)	P(2)-C(31)-C(32)	122.7(3)
Rh(1)-C(1)-O	135.3 (6)	P(2)-C(31)-C(36)	117.3(3)
Rh(2)-C(1)-O	135.3 (6)	P(2)-C(41)-C(42)	118.7(3)
P(1)-C(2)-P(2)	111.0 (4)	P(2)-C(41)-C(46)	121.2(3)
P(3)-C(3)-P(4)	109.9 (4)	P(3)-C(51)-C(52)	120.4(4)
Rh(1)-P(1)-C(2)	112.6 (3)	P(3)-C(51)-C(56)	119.6(4)
Rh(2)-P(2)-C(2)	114.1 (2)	P(3)-C(61)-C(62)	116.2(4)
Rh(1)-P(3)-C(3)	114.0 (2)	P(3)-C(61)-C(66)	123.8(4)
Rh(1)-P(4)-C(3)	112.1 (2)	P(4)-C(71)-C(72)	118.7(3)
Rh(1)-P(1)-C(11)	115.4 (2)	P(4)-C(71)-C(76)	121.2(3)
Rh(1)-P(1)-C(21)	115.6 (2)	P(4)-C(81)-C(82)	117.4(3)
Rh(2)-P(2)-C(31)	108.0 (2)	P(4)-C(81)-C(86)	122.6(3)
Rh(2)-P(2)-C(41)	121.8 (2)		

## Torsion Angles

P(1)-Rh(1)-Rh(2)-P(2)	- 5.42(7)	C(2)-P(1)-Rh(1)-C(1)	- 17.9 (4)
P(1)-Rh(1)-Rh(2)-P(4)	170.87(7)	C(2)-P(2)-Rh(2)-C(1)	28.3 (4)
P(2)-Rh(2)-Rh(1)-P(3)	-172.97(7)	C(3)-P(3)-Rh(1)-C(1)	17.6 (4)
P(3)-Rh(1)-Rh(2)-P(4)	3.32(8)	C(3)-P(4)-Rh(2)-C(1)	- 24.8 (4)
C(11)-P(1)-Rh(1)-Br(1)	73.8 (2)	C(11)-P(1)-P(2)-C(31)	2.6 (3)
C(21)-P(1)-Rh(1)-Br(1)	- 48.7 (2)	C(11)-P(1)-P(3)-C(61)	- 6.5 (3)
C(31)-P(2)-Rh(2)-Br(2)	- 65.2 (2)	C(21)-P(1)-P(2)-C(41)	5.2 (4)
C(41)-P(2)-Rh(2)-Br(2)	54.1 (2)	C(21)-P(1)-P(3)-C(51)	- 9.3 (3)
C(51)-P(3)-Rh(1)-Br(1)	40.7 (3)	C(31)-P(2)-P(4)-C(71)	- 3.0 (3)
C(61)-P(3)-Rh(1)-Br(1)	- 80.0 (2)	C(41)-P(2)-P(4)-C(81)	- 6.6 (3)
C(71)-P(4)-Rh(2)-Br(2)	63.1 (2)	C(51)-P(3)-P(4)-C(81)	30.1 (4)
C(81)-P(4)-Rh(2)-Br(2)	- 59.7 (2)	C(61)-P(3)-P(4)-C(71)	19.1 (3)

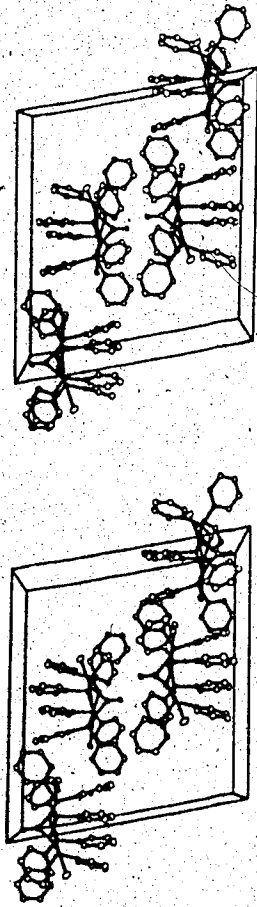


Figure 19. Cell Packing Diagram of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ .

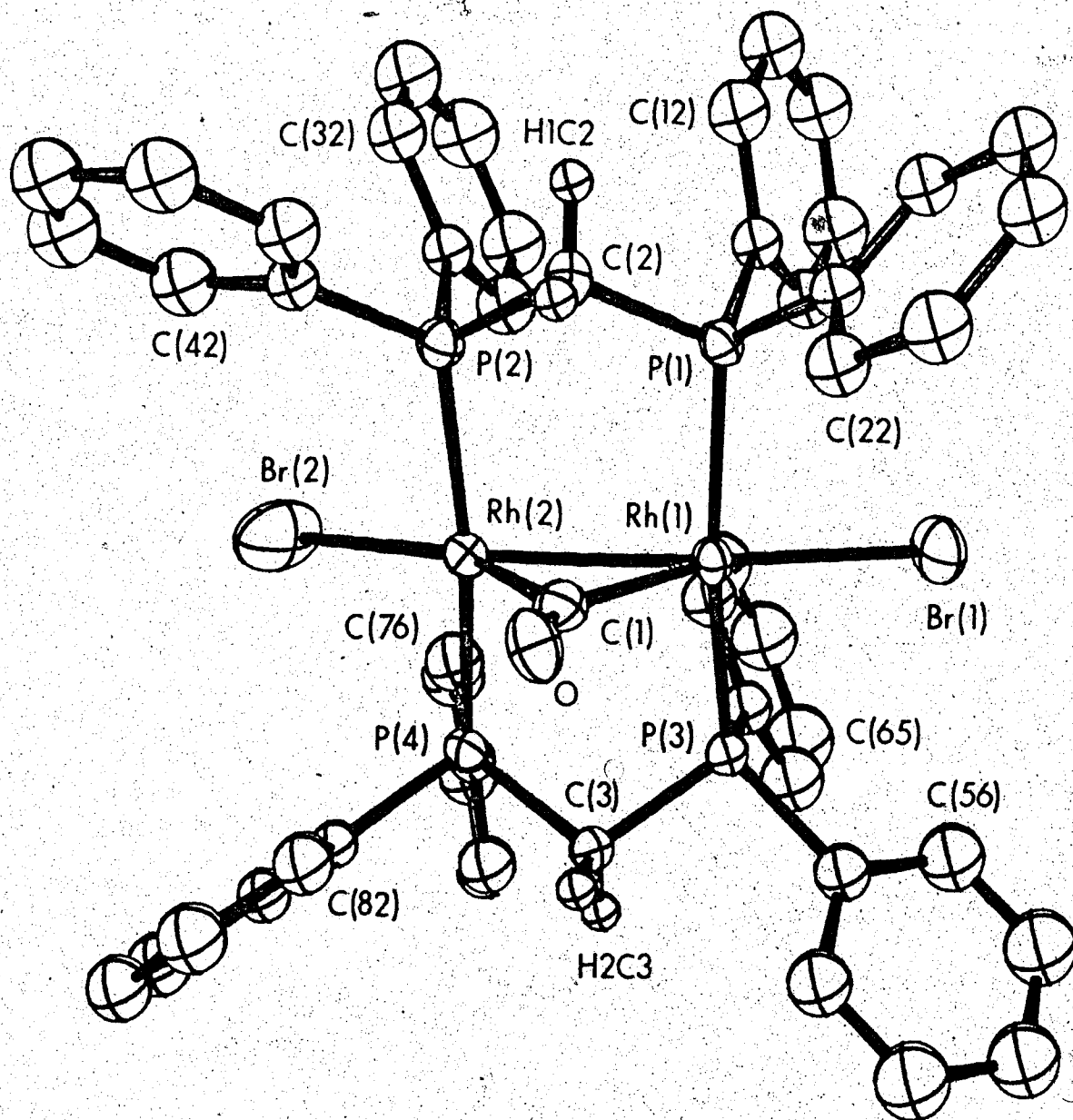


Figure 20. A Perspective View of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ .

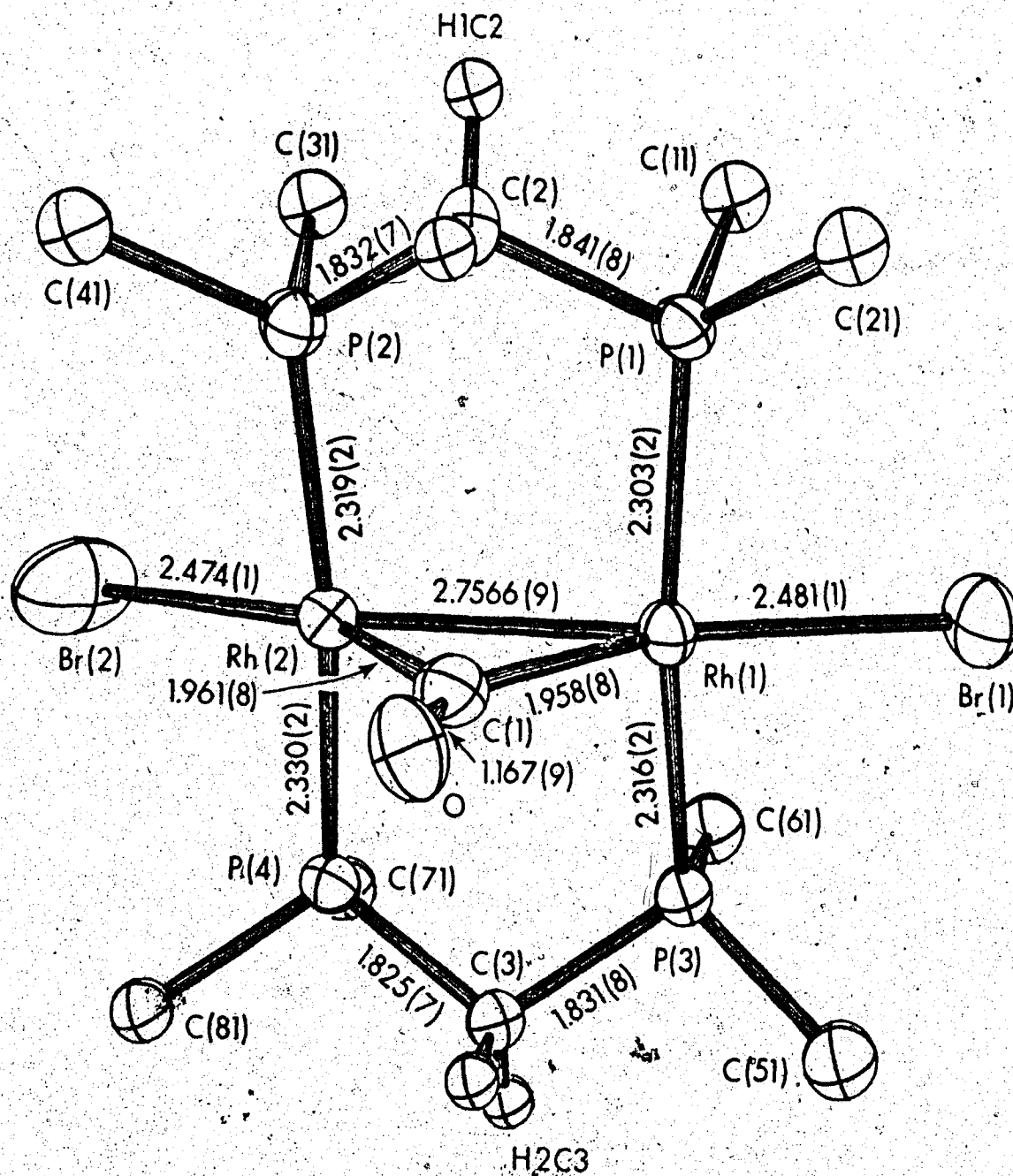


Figure 21. The Inner Coordination Sphere of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$ .

## DESCRIPTION OF STRUCTURE

The coordination about each rhodium atom is quasi-trigonal bipyramidal. Two transoid DPM ligands bridge the Rh atoms in the axial positions with the bridging carbonyl ligand, a terminal bromo ligand on each Rh atom and a formal Rh-Rh bond completing coordination in the equatorial plane. The resulting distorted "A-frame" geometry is similar to that observed in  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]^{96}$  (Chapter IV). The distortions in the "A-frame" geometry arise due to steric interactions between the terminal bromo ligands and the phenyl rings of the DPM ligands (Table 32) and because of the presence of a metal-metal bond, both resulting in a flattening of the "A" configuration. Angles about each Rh atom in the equatorial plane clearly show the distortions from trigonal bipyramidal coordination (Rh-Rh-Br, Rh-Rh-C(1), and Br-Rh-C(1); 167.06(4), 45.3(2) and 147.6(2)°, respectively).

The Rh-Br distances of 2.481(1) and 2.474(1)Å are not unusual and compare well with other determinations.<sup>149,150</sup> Within the Rh-DPM framework most parameters are as expected. The Rh-P distances (average 2.317(11)Å) and the P-C distances both methylene and phenyl (average, 1.833(7) and 1.832(8)Å, respectively) compare well with other determinations.<sup>35,89,96,120,126,142</sup> The Rh-P vectors as viewed down the Rh-Rh axis are slightly staggered (see P-Rh-Rh-P torsion angles in Table 33 and least-squares planes in

Table 31). This skewing of the Rh-DPM framework results in phenyl rings 3 and 6 being forced into the open coordination site opposite the carbonyl ligand giving rise to close contacts between Rh and the ortho hydrogen atoms (2.65 and 2.81 Å). An almost identical skewing was observed in the chloro/SO<sub>2</sub> analogue, [Rh<sub>2</sub>Cl<sub>2</sub>(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>]<sup>96</sup> (Chapter IV). The Rh-P-C angles with the exceptions of those for rings 4 and 5 are close to the expected tetrahedral values. In contrast, the Rh-P-C angles involving ring 4 and 5 (121.8(2)° and 123.1(2)°, respectively) are significantly larger than the expected tetrahedral values. These distortions seem to arise from steric interactions between the bromo ligand and the phenyl rings, as evidenced by the short Br-H distances involving these rings (Br(1) - H(56) = 3.15 Å and Br(1) - H(42) = 2.75 Å) which are less than the sums of the van der Waal's radii.<sup>112</sup> In the structure of [Rh<sub>2</sub>Cl<sub>2</sub>(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>]<sup>96</sup> where the bromo ligand is replaced by the less bulky chloro ligand these distortions are somewhat less pronounced, with a maximum value for the Rh-P-C angle of 118.9(2)°. The bromo ligands in the present compound, are staggered with respect to the DPM phenyl groups, in order to minimize nonbonded contacts between these groups. This staggering is evident in the phenyl-P-Rh-Br torsion angles which range from 40.7(3)° to 80.0(2)° (Table 33).

Formally the present compound contains a Rh-Rh single bond as suggested by several structural parameters:

i) the Rh-Rh distance of  $2.7566(9)\text{\AA}$  falls within the range previously reported for similar Rh-Rh bond species ( $2.617(3)$  -  $2.8415(7)\text{\AA}$ )<sup>35,129-133</sup> and can be contrasted to the distances of  $3.1520(8)$  and  $3.155(4)\text{\AA}$ , observed in the "A-frame" species  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  (Chapter II) and  $[\text{Rh}_2(\text{CO})_2(\mu\text{-S})(\text{DPM})_2]$ ,<sup>89</sup> respectively, where no formal metal-metal bond is present; ii) the Rh-C-Rh bond angle of  $89.4(4)^\circ$  compares well with other determinations in which a carbonyl ligand bridges a metal-metal bond,<sup>35,130-133</sup> and is significantly smaller than the values of  $119(3)^\circ$ ,  $106(3)^\circ$  and  $116.4(6)^\circ$  observed in  $[\text{Pd}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$ ,<sup>32</sup>  $[\text{Pt}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$ <sup>41</sup> and  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\mu\text{-DMA})(\text{DPM})_2]$ ,<sup>42</sup> respectively, where no metal-metal bond is present; iii) the Rh-Rh separation is significantly less than the P...P intraligand separations of  $3.026(3)$  and  $2.992(3)\text{\AA}$  as is usually observed in these systems when a Rh-Rh bond is present.<sup>35</sup>

Although the above parameters suggest a direct metal-metal bond, this formulation is by no means unambiguous. Recent molecular orbital calculations<sup>151</sup> on carbonyl bridged species with short metal-metal distances have shown that in some cases no metal-metal bond is actually present even though the structural parameters suggest otherwise. Furthermore, these calculations have been substantiated by experimental differential electron density determinations<sup>152</sup> on the compounds in question showing no significant build-up of electron density along the metal-metal axis.

The carbonyl ligand bridges the two Rh atoms symmetrically as evidenced by the Rh-C distances of 1.958(8) and 1.961(8) Å. These distances are significantly shorter than those observed in other Rh systems containing bridging carbonyl ligands where the values of 2.104(7) and 2.034(7) Å, observed in  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2][\text{BPh}_4]$ ,<sup>35</sup> are more typical. Instead, the observed distances are comparable to the values of 1.90(6) and 1.97(9) Å obtained in the Pd<sup>32</sup> and Pt<sup>41</sup> analogues  $[\text{M}_2\text{Cl}_2(\mu\text{-CO})(\text{DAM})_2]$ , (M = Pd, Pt) and that of 1.974(7) observed in  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\mu\text{-DMA})(\text{DPM})_2]$ .<sup>42</sup> It is notable that these distances correspond to "ketonic" carbonyl species which show low values for  $\nu(\text{CO})$  in the infrared spectrum similar to that observed for the present compound. It is also relevant that the analogous  $\text{SO}_2$  species  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  has short Rh-S bonds and a low value for  $\nu(\text{SO})$  in the infrared spectrum (Chapter IV).

In the title compound the C(1)-O distance is not as long as one might expect based on the low  $\nu(\text{CO})$ , but rather is comparable to that observed in "normal" bridging carbonyls which have  $\nu(\text{CO})$  ca.  $100\text{ cm}^{-1}$  higher. However, carbonyl C-O distances are not overly sensitive to such changes owing to the relatively large uncertainty in the atomic positions. Therefore the present distance is, within experimental error, comparable to the analogous distances in the "ketonic" carbonyl species of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\mu\text{-DMA})(\text{DPM})_2]$ <sup>42</sup> and  $[\text{Pd}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$ <sup>32</sup> where the  $\nu(\text{CO})$  values of  $1700$  and  $1720\text{ cm}^{-1}$ , respectively are ob-



served. Applying a riding motion correction the present C(1)-O distance (atom O riding on C(1)) yields a corrected value of 1.192(9) Å which is closer to the value we had expected based on spectral parameters.

### DISCUSSION

The structural determination of  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  has unambiguously established it to be a monocarbonyl species having a formal Rh-Rh bond and not the alternate dicarbonyl species. The spectral parameters are consistent with both formulations (mono and dicarbonyl species), but the reaction of the compound with  $\text{SO}_2$ , yielding a dicarbonyl product, at first glance actually favours the dicarbonyl formulation. Prompted by the present structural characterization however, a reinvestigation of the  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra during the slow stepwise addition of  $\text{SO}_2$  indicates the dicarbonyl species results from CO transfer from one monocarbonyl species to another (see Chapter V). A somewhat analogous, facile CO transfer has been reported<sup>35a,91</sup> between  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  and  $[\text{Rh}_2(\text{CO})_2(\mu\text{-CO})(\mu\text{-Cl})(\text{DPM})_2]^+$ . These results clearly indicate the need for further structural and spectral characterizations of related complexes in order to yield the needed correlations between their structural and spectral parameters.

The complex,  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  is only the second structurally characterized example with rhodium<sup>145</sup> in which a carbonyl ligand occupies the bridging site in

preference to the halide ligand. Generally the reverse is true,<sup>153</sup> yet in binuclear DPM-,<sup>42,125</sup> DAM-<sup>32,41</sup> and analogous diphosphazane-bridged<sup>145</sup> complexes of the Group VIII metals several complexes have now been characterized with bridging CO and terminal halide ligands. The closely related, SO<sub>2</sub> bridged species, [Rh<sub>2</sub>Cl<sub>2</sub>(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>] is also anomalous in this regard having bridging SO<sub>2</sub> and terminal chloro groups (Chapter IV). It seems that in these complexes there is a strong tendency for the better π-acceptor ligand to enter the bridging site, even when initial attack by this ligand is terminal. In the bridging site the π-acceptor ligand can accept electron density from both electron rich metals, which in the present complex would account for the low value of ν(CO) and the short rhodium carbonyl distances. In addition the build-up of electron density on the carbonyl ligand, resulting from the large degree of back donation from the metal is also reflected in the low field chemical shift (227.5 ppm) of the <sup>13</sup>C carbonyl resonance. The trend in spectral parameters with increasing metal carbonyl back bonding is seen clearly in the series of closely related complexes [Rh<sub>2</sub>(CO)<sub>2</sub>(μ-CO)(μ-Cl)(DPM)<sub>2</sub>]<sup>+</sup>, [Rh<sub>2</sub>I(CO)(μ-CO)(DPM)<sub>2</sub>][I] and [Rh<sub>2</sub>Br<sub>2</sub>(μ-CO)(DPM)<sub>2</sub>], where the observed <sup>13</sup>C chemical shifts for the bridging carbonyl ligands (203.2,<sup>154</sup> 212.8<sup>154</sup> and 227.5 ppm, respectively) directly parallel the corresponding ν(CO) values (1850, 1810 and 1745 cm<sup>-1</sup>,

respectively).<sup>155</sup> In contrast however, the "ketonic" carbonyl complexes,  $[\text{Rh}_2\text{X}_2(\mu\text{-CO})(\mu\text{-acetylene})(\text{DPM})_2]$  ( $\text{X} = \text{Cl}, \text{Br}, \text{I}$ ), which have even lower values of  $\nu(\text{CO})$  of *ca.* 1700  $\text{cm}^{-1}$  have relatively high field  $^{13}\text{C}$  shifts of *ca.* 190 ppm.<sup>42</sup> It is unclear at this time why the "ketonic" carbonyl species have such different  $^{13}\text{C}$  chemical shifts from the present compound when the carbonyl stretching frequencies are comparable, but it is clear that the use of spectral parameters to assign the mode of carbonyl bonding is fraught with difficulties, at least until more complete spectral and structural correlations are available.

## CHAPTER VII.

### Carbon Disulfide Chemistry and the the Structure of $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$

#### INTRODUCTION

Much of the recent interest in carbon disulfide chemistry stems from the close similarity of this molecule to the less reactive carbon dioxide molecule. Few species, however containing either of these ligands have been structurally characterized.<sup>45-47,156-160</sup> For the  $\text{CS}_2$  molecule, the commonest coordination mode, and one of the bonding modes also observed for the analogous  $\text{CO}_2$  molecule,<sup>160</sup> has the  $\text{CS}_2$  molecule bound to the metal in a side-on manner, through the carbon atom and one of the sulfur atoms (see Chapter I).<sup>45,156-159</sup>

For rhodium and iridium several  $\text{CS}_2$  containing complexes have been prepared<sup>48,161</sup> but until recently none had been structurally characterized.<sup>162</sup> In several of these complexes the  $\text{C},\text{S}-\eta^2$  bonding mode of the  $\text{CS}_2$  molecules had been inferred based on analogies with other transition metal complexes<sup>48,161</sup> even though the C-S stretching frequencies observed were typically *ca.*  $100\text{ cm}^{-1}$  lower than those observed in structurally confirmed complexes.<sup>3</sup> These low values of  $\nu(\text{CS})$  suggest that the  $\text{CS}_2$  molecule may adopt another coordination geometry in these rhodium and iridium complexes. One possibility which must be considered in-

volves the condensation of the  $\text{CS}_2$  molecules. Certainly rhodium has previously displayed a tendency of condensing sulfur containing ligands, for example in  $[\text{RhCl}(\text{PPh}_3)_2(\text{PhCONCS})_2]$ <sup>163</sup> and  $[\text{RhCl}(\text{PPh}_3)_2(\text{C}_2\text{H}_5\text{OCONCS})_3]$ <sup>164</sup> where two molecules of  $\text{PhCONCS}$  and three molecules of  $\text{C}_2\text{H}_5\text{OCONCS}$ , respectively, are condensed at the metal centres. Significantly, one of the few structurally characterized " $\text{CO}_2$  complexes" actually contains a  $\text{C}_2\text{O}_4$  fragment resulting from the condensation of two  $\text{CO}_2$  molecules.<sup>50</sup> The  $\text{CO}$  stretching frequencies for this species are  $25\text{--}75\text{ cm}^{-1}$  lower than those in a typical  $\text{C},\text{O}-\eta^2$  bond species.<sup>160</sup> Furthermore, while this work was in progress the structural determination of  $[\text{Rh}(\text{C}_2\text{S}_4)(\eta^5\text{-C}_5\text{H}_5)(\text{PMe}_3)]$ <sup>162</sup> indicated that the  $\text{C}_2\text{S}_4$  fragment was bound in an analogous manner to the above  $\text{C}_2\text{O}_4$  moiety and again the values of  $\nu(\text{CS})$  for this species were low.

In view of the obvious lack of structural information available on  $\text{CS}_2$  complexes, the present study was undertaken in order to form a much needed basis for spectral and structural correlations in these complexes and to gain a better understanding of transition metal activation of  $\text{CS}_2$  and related molecules.

#### EXPERIMENTAL

All reactions were performed under a dinitrogen atmosphere using degassed solvents.

Preparation of  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$

A suspension of 0.200 g (0.182 mmol) of *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  (1) in 25 mL of  $\text{CH}_2\text{Cl}_2$  was treated with 10 mL of  $\text{CS}_2$  and allowed to react for 24 h. To the resulting red solution was added 25 mL of diethyl ether to induce crystallization. This complex may also be prepared in a manner analogous to that shown above, from the reaction of  $\text{CS}_2$  with  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$ .

Spectroscopic Studies

A solution was prepared by dissolving 0.100 g (0.072 mmol) of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  (2) in 4 mL of  $\text{CD}_2\text{Cl}_2$  in a 10 mm NMR tube. The  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum was recorded at 233 K. Subsequent  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra were then recorded after each 1.5  $\mu\text{L}$  (0.035 mmol) addition of  $\text{CS}_2$  until all of 2 had been converted to  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$  (3). In addition to resonances assignable to 2 ( $\delta = 19.7$  ppm;  $|^1J_{\text{Rh-P}} + ^xJ_{\text{Rh-P}}| = 115.9$  Hz)<sup>101</sup> and 3 ( $\delta = 7.5$  ppm; AA'BB'XY multiplet), two additional resonances due to symmetric species at  $\delta = 15.7$  ppm ( $|^1J_{\text{Rh-P}} + ^xJ_{\text{Rh-P}}| = 116.5$  Hz) and  $\delta = 14.3$  ppm ( $|^1J_{\text{Rh-P}} + ^xJ_{\text{Rh-P}}| = 98.2$  Hz) were also observed at intermediate times in the reaction. Similarly the  $^{13}\text{C}\{^{31}\text{P}\{^1\text{H}\}\}$  NMR spectra were monitored using exactly the same technique and starting with  $[\text{Rh}_2\text{Cl}_2(\mu\text{-}^{13}\text{CO})(\text{DPM})_2]$ . Carbonyl resonances assignable to 2 ( $\delta = 229.0$  ppm; triplet;  $|J_{\text{Rh-C}}| = 44.9$  Hz), 3 ( $\delta = 191.5$  ppm; doublet;  $|J_{\text{Rh-C}}| = 69.1$  Hz) and a third species ( $\delta = 186.5$  ppm; doublet;

$|J_{\text{Rh-C}}| = 80.1 \text{ Hz}$ ) were observed.

Infrared spectra were obtained in an analogous manner, by recording the solution spectrum after each stepwise addition of 7  $\mu\text{L}$  (0.116 mmol) of  $\text{CS}_2$  to a  $\text{CH}_2\text{Cl}_2$  solution of 2 (0.500 g, 0.465 mmol) in 30 mL. Unfortunately the  $\text{CS}_2$  stretching region was obscured by DPM and free  $\text{CS}_2$  bands. In the bridging carbonyl region only one band was observed, which was assignable to 2 ( $\nu(\text{CO}) = 1750 \text{ cm}^{-1}$ ). In addition, two vibrations were observed in the terminal carbonyl region; the one at  $2030 \text{ cm}^{-1}$  increased in intensity throughout the experiment and was assigned to species 3, and the second at  $1990 \text{ cm}^{-1}$  was observed at intermediate times in the experiment.

#### Crystallization of $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$

To a solution of 0.100 g (0.0798 mmol) of 3 in 10 mL of  $\text{CH}_2\text{Cl}_2$  was added 2 mL of  $\text{CS}_2$  and 7 mL of diethyl ether. Crystallization was induced from this solution by slow cooling, yielding red crystals. An infrared spectrum ( $\nu(\text{CO}) = 2040(\text{sh}), 2020(\text{s}) \text{ cm}^{-1}$ ;  $\nu(\text{C-S}) = 1050(\text{m}), 995(\text{sh}), 980(\text{s}) \text{ cm}^{-1}$ ) verified that it was species 3.

#### X-Ray Data Collection

Red crystals of  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$  were mounted in glass capillaries. Preliminary film data showed that these crystals were of only mediocre quality, however repeated attempts to obtain crystals of better quality failed.

The structural investigation was therefore continued on the original crystals. These crystals belong to the monoclinic system with extinctions ( $h0l$ ,  $l$  odd;  $0k0$ ,  $k$  odd) characteristic of the centrosymmetric space group  $P2_1/c$ . The density calculation, and the cell parameters, indicated that  $Z = 8$ , revealing that two independent dimers per asymmetric unit were present. Therefore, a cell reduction<sup>102</sup> was performed to rule out the possibility that the crystals might belong to a system of higher symmetry. The cell reduction confirmed the  $P2_1/c$  cell as the reduced cell and the solution of the structure verified this, showing that the two independent dimers in the asymmetric unit have slight but significant differences in their geometries (vide infra).

Data collection was carried out as previously described in Chapter II. Pertinent crystal and intensity collection data are presented in Table 34. Data collection was suspended at  $2\theta = 100^\circ$ , owing to the lack of diffracted intensity beyond this point. During data collection a clear colorless liquid was observed condensing on the inside of the capillary. However, by the time data collection had finished this liquid had disappeared (presumably through a pinhole in the capillary) so no identification of this liquid was possible.

### Solution of Structure

Since species 3 crystallized with two independent dimers per asymmetric unit, and therefore has four inde-



Table 34. Summary of Crystal Data and Intensity Collection  
for  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$

Compound	$[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$																								
Formula	$\text{C}_{53}\text{H}_{44}\text{Cl}_2\text{O}_1\text{P}_4\text{Rh}_2\text{S}_4$																								
Formula Weight																									
Cell Parameters																									
a	22.311(3) Å																								
b	22.843(3) Å																								
c	22.828(3) Å																								
$\beta$	115.21(1)°																								
V	10526 Å <sup>3</sup>																								
Z	8																								
Density	1.547 g·cm <sup>-3</sup> (calc'd.) 1.56(2) g·cm <sup>-3</sup> (expt'l. by flotation)																								
Space Group	$\text{C}_{2h}^5 - \text{P}2_1/c$																								
Crystal Dimensions	0.586 x 0.211 x 0.629																								
Crystal Volume	0.0458 mm <sup>3</sup>																								
Crystal Faces (and distances from an arbitrary origin within the crystal (mm))	<table border="0"> <tbody> <tr> <td>1</td> <td>0</td> <td>0</td> <td>(0.256)</td> </tr> <tr> <td><math>\bar{1}</math></td> <td>0</td> <td><math>\bar{1}</math></td> <td>(0.203)</td> </tr> <tr> <td><math>\bar{5}</math></td> <td>0</td> <td><math>\bar{2}</math></td> <td>(0.252)</td> </tr> <tr> <td><math>\bar{1}</math></td> <td>0</td> <td>1</td> <td>(0.182)</td> </tr> <tr> <td>0</td> <td><math>\bar{1}</math></td> <td>0</td> <td>(0.105)</td> </tr> <tr> <td>0</td> <td><math>\bar{1}</math></td> <td>0</td> <td>(0.105)</td> </tr> </tbody> </table>	1	0	0	(0.256)	$\bar{1}$	0	$\bar{1}$	(0.203)	$\bar{5}$	0	$\bar{2}$	(0.252)	$\bar{1}$	0	1	(0.182)	0	$\bar{1}$	0	(0.105)	0	$\bar{1}$	0	(0.105)
1	0	0	(0.256)																						
$\bar{1}$	0	$\bar{1}$	(0.203)																						
$\bar{5}$	0	$\bar{2}$	(0.252)																						
$\bar{1}$	0	1	(0.182)																						
0	$\bar{1}$	0	(0.105)																						
0	$\bar{1}$	0	(0.105)																						
Temperature	20°C																								
Radiation	$\text{CuK}\alpha$ ( $\lambda=1.540562$ Å) filtered with 0.5 mil thick nickel foil																								
$\mu$	90.85																								
Range in Absorption Correction Factors	0.081 - 0.230																								
Receiving Aperture	6 x 6 mm, 30 cm from the crystal																								

Table 34, continued

Takeoff Angle	6.2°
Scan Speed	2° in 2θ/min
Scan Range	1.00° below K <sub>α1</sub> to 1.00° above K <sub>α2</sub>
Background Counting Time	10s (2° < 2θ < 80°) 20s (80° < 2θ < 100°)
2θ limits	2° < 2θ < 100°
2θ limits for centered reflections	50° < 2θ < 60°
Final number of variables	337
Unique Data Collected	11195
Unique Data Used ( $F_o^2 \geq 3\sigma(F_o^2)$ )	5929
Error in observation of unit weight	2.472
R	0.114
R <sub>w</sub>	0.145

pendent rhodium atoms, structure solution was initially attempted using the direct methods program MULTAN.<sup>148</sup> However, efforts at solving the structure using MULTAN failed after repeated attempts, using between 500 and 700 reflections having the highest E's and generating between 2000 to 5000 unique phase relationships. In all solutions generated by MULTAN the same molecular orientations (for Rh and P) kept recurring, only with different relative positions of the dimers. This problem (of finding the molecular framework but failing to fix the origin) is not uncommon with MULTAN and is not unexpected given that in this structure we were attempting to push MULTAN far beyond its recommended limits. It is generally recommended to use about seven phase relationships per reflection and seven reflections per atom, whereas we were using at maximum 5.3 reflections per atom and generating 7.1 phase relationships per reflection. In addition, structures that require more than 500 reflections are generally too difficult for MULTAN to solve.

Our previous experience with these systems suggested that the Patterson map would be extremely difficult to interpret owing to vector build-up, especially considering that two molecules per asymmetric unit were present. This suspicion was confirmed by the calculated Patterson map, which showed severe Rh-Rh and Rh-P vector build-up. The top weighted vector, for example, at (0.44, 0.50, 0.44) was equal to approximately eleven times a singly weighted Rh-Rh

vector. As a result of this vector build-up in the Patterson map even using the Rh-P frameworks found in MULTAN, again the origin could not be uniquely defined. Therefore, one of the dimers, obtained from MULTAN, was arbitrarily chosen and its Rh-P framework was shifted to all possible positions consistent with the Patterson map, maintaining the orientation given by MULTAN. Subsequent full matrix least-squares and electron density difference maps on each possible solution established that the solution having Rh(A1) at (0.77, 0.14, 0.02) and Rh(A2) at (0.78, 0.02, 0.02) was considerably better than the others. In this solution, including the four associated P atoms,  $R = 0.49$  and  $R_w = 0.61^{121}$  compared to values of near 0.53 and 0.63 for  $R$  and  $R_w$ , respectively, for other solutions. Furthermore, with this solution the Rh-P framework of the second dimer was observed at a position consistent with the Patterson map (other possible solutions did not yield this framework). The remaining atoms were located from subsequent least-squares calculations and electron density difference maps. Anomalous dispersion terms<sup>108</sup> for Rh, P, Cl and S were included in  $F_c$ . The phenyl carbon atoms were refined as rigid groups and hydrogen atoms were included as fixed contributions and not refined. All other nongroup atoms except hydrogens were refined with isotropic thermal parameters. An anisotropic refinement of, at least the heavy atoms (Rh, Cl, S and P), would have been appropriate on the

basis of the residual electron density observed around these atoms (range  $-3.11$  to  $2.69 \text{ e}/\text{\AA}^3$ ). However, this was not attempted due to the extremely high cost associated with refining these atoms anisotropically.

At this point an electron density difference map revealed the presence of an unresolved tunnel of electron density in the area enclosed by the phenyl ring of P(A3), P(A4), P(B2), and P(B4). Attempts to fit this area to  $\text{CS}_2$ ,  $\text{CH}_2\text{Cl}_2$  or  $(\text{C}_2\text{H}_5)_2\text{O}$  molecules were unsuccessful, however. Unreasonable geometries and thermal parameters resulted and no significant improvement in the crystallographic residuals was observed. The poorly resolved nature of this electron density probably results in part from the loss in solvent of crystallization which was observed during data collection (vide supra) and explains the poor diffraction quality of the crystals and the slight decrease in intensities of the standard reflections during data collection.

The final model with 337 parameters varied converged to  $R = 0.114$  and  $R_w = 0.145$ .<sup>121</sup> At this point an electron density difference map showed the highest 20 peaks ( $2.69 - 1.00 \text{ e}/\text{\AA}^3$ ) were in the vicinities of the heavy atoms and the tunnel of electron density. A typical carbon atom of an earlier syntheses had an electron density of  $3.2 \text{ e}/\text{\AA}^3$ .

## Results

The positional and thermal parameters for the individual isotropic atoms, rigid group atoms and idealized hydro-

gen atoms are given in Tables 35, 36 and 37, respectively. Least squares plane calculations are presented in Table 38 and selected bond lengths and angles are shown in Tables 39 and 40, respectively. A listing of observed and calculated structure amplitudes is available.<sup>110</sup>

A stereoview of both dimers is shown in Figure 22. Figure 23 shows a perspective view of dimers A and B. Phenyl carbon atoms are labelled sequentially around the ring starting at the carbon bound to phosphorus. The equatorial planes for  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$  are shown in Figure 24 and include relevant bond lengths.

TABLE 35. Positional and Thermal Parameters For The Nongroup Atoms of  $[\text{Rh}_2\text{C}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$ .

Atom	x	y	z	B(A <sup>1</sup> )	Atom	x	y	z	B(A <sup>1</sup> )
Rh(A1)	0.76980(9)	0.14301(8)	0.01950(9)	3.93(5)	P(A3)	0.8667(4)	0.1538(3)	0.1173(4)	4.8(2)
Rh(A2)	0.7819(1)	0.02064(8)	0.0180(1)	4.06(5)	P(A4)	0.8686(3)	0.0216(3)	0.1226(3)	4.5(2)
Rh(B1)	0.32896(9)	0.10029(8)	0.59006(9)	4.03(5)	P(B1)	0.3452(4)	0.2008(3)	0.5886(3)	4.6(2)
Rh(B2)	0.2210(1)	0.09592(9)	0.4676(1)	4.65(5)	P(B2)	0.2181(4)	0.1984(3)	0.4604(4)	5.4(2)
C1(A1)	0.7146(3)	0.1599(3)	0.0895(3)	5.1(1)	P(B3)	0.3242(3)	-0.0010(3)	0.6054(3)	4.3(1)
C1(A2)	0.8062(4)	-0.0864(3)	0.0166(4)	6.5(2)	P(B4)	0.2072(4)	-0.0069(3)	0.4692(4)	4.9(2)
C1(B1)	0.2562(3)	0.1228(3)	0.6429(3)	5.3(2)	O(A1)	0.6919(9)	-0.0050(8)	0.0811(9)	6.8(5)
C1(B2)	0.1467(4)	0.0905(3)	0.3476(4)	6.7(2)	O(B1)	0.118(1)	0.101(1)	0.516(1)	11.3(8)
S(A1)	0.7775(3)	0.2436(3)	0.0021(3)	4.9(2)	C(A1)	0.725(1)	0.010(1)	0.058(1)	4.8(6)
S(A2)	0.8120(5)	0.3064(4)	-0.0926(5)	8.3(2)	C(B1)	0.147(1)	0.102(1)	0.492(1)	5.8(7)
S(A3)	0.8279(4)	0.1810(3)	-0.0821(4)	5.3(2)	C(A2)	0.670(1)	0.081(1)	-0.130(1)	4.6(5)
S(A4)	0.8439(3)	0.0611(3)	-0.0354(3)	4.6(2)	C(A3)	0.875(1)	0.089(1)	0.169(1)	3.8(5)
S(B1)	0.4355(3)	0.0967(3)	0.6764(3)	4.7(1)	C(B2)	0.266(1)	0.238(1)	0.537(1)	6.2(7)
S(B2)	0.5694(4)	0.0879(4)	0.6791(4)	7.3(2)	C(B3)	0.248(1)	-0.036(1)	0.554(1)	5.5(6)
S(B3)	0.4554(3)	0.0835(3)	0.5558(3)	5.2(2)	C(A4)	0.802(1)	0.247(1)	-0.058(1)	5.1(6)
S(B4)	0.3210(3)	0.0869(3)	0.4536(3)	5.1(2)	C(A5)	0.816(1)	0.128(1)	-0.032(1)	4.9(6)
P(A1)	0.6672(3)	0.1356(3)	-0.0715(3)	4.3(1) <sup>a</sup>	C(B4)	0.488(1)	0.089(1)	0.639(1)	5.1(6)
P(A2)	0.7001(3)	0.0106(3)	-0.0892(3)	4.1(1)	C(B5)	0.370(1)	0.090(1)	0.531(1)	4.0(5)

<sup>a</sup> Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

TABLE 36. Derived Parameters For the Rigid Group Atoms of [Rh2C12(CO)(C2S4)(DPM)2].

Atom	X	Y	Z	B(A')	Atom	X	Y	Z	B(A')
C(A11)	0.6399(9)	0.2021(7)	-0.121(1)	3.9(5)	C(B11)	0.3670(8)	0.2404(8)	0.6641(7)	4.2(5)
C(A12)	0.637(1)	0.2082(7)	-0.183(1)	6.6(7)	C(B12)	0.3828(9)	0.2127(5)	0.7231(9)	5.5(6)
C(A13)	0.610(1)	0.2586(9)	-0.2187(7)	7.8(9)	C(B13)	0.4022(8)	0.2456(8)	0.7796(7)	6.3(7)
C(A14)	0.5861(9)	0.3030(7)	-0.193(1)	7.5(8)	C(B14)	0.4057(8)	0.3063(8)	0.7770(7)	5.4(6)
C(A15)	0.589(1)	0.2969(7)	-0.131(1)	7.6(8)	C(B15)	0.3899(9)	0.3341(5)	0.7179(9)	9.0(9)
C(A16)	0.616(1)	0.2465(9)	-0.0949(7)	4.6(6)	C(B16)	0.3706(8)	0.3012(8)	0.6615(7)	6.3(7)
C(A21)	0.588(2)	0.1139(8)	-0.0710(7)	4.1(5)	C(B21)	0.410(2)	0.2249(8)	0.566(4)	4.1(5)
C(A22)	0.588(2)	0.0893(8)	-0.015(2)	5.5(7)	C(B22)	0.398(4)	0.2307(8)	0.501(2)	6.6(7)
C(A23)	0.528(2)	0.0721(8)	-0.015(2)	6.4(7)	C(B23)	0.449(5)	0.2450(8)	0.484(3)	4.7(6)
C(A24)	0.469(2)	0.0795(8)	-0.0695(7)	6.8(7)	C(B24)	0.513(2)	0.2534(8)	0.532(4)	6.7(7)
C(A25)	0.469(2)	0.1041(8)	-0.125(2)	7.6(8)	C(B25)	0.525(4)	0.2476(8)	0.597(2)	7.6(8)
C(A26)	0.528(2)	0.1213(8)	-0.126(2)	5.2(6)	C(B26)	0.474(5)	0.2334(8)	0.614(3)	5.1(6)
C(A31)	0.6253(8)	-0.0310(7)	-0.1010(6)	3.4(5)	C(B31)	0.2404(9)	0.2368(8)	0.4035(7)	4.7(6)
C(A32)	0.564(1)	-0.0191(6)	-0.1521(9)	5.3(6)	C(B32)	0.2494(9)	0.2972(8)	0.4078(7)	5.8(7)
C(A33)	0.5088(7)	-0.0521(7)	-0.1598(8)	5.0(6)	C(B33)	0.2666(9)	0.3263(6)	0.3636(9)	7.9(9)
C(A34)	0.5145(8)	-0.0970(7)	-0.1165(6)	5.6(6)	C(B34)	0.2748(9)	0.2951(8)	0.3152(7)	6.5(7)
C(A35)	0.576(1)	-0.1088(6)	-0.0654(9)	5.3(6)	C(B35)	0.2658(9)	0.2347(8)	0.3109(7)	6.1(7)
C(A36)	0.6310(7)	-0.0759(7)	-0.0576(8)	5.1(6)	C(B36)	0.2485(9)	0.2055(6)	0.3551(9)	6.0(7)
C(A41)	0.722(2)	-0.0274(9)	-0.149(2)	4.5(5)	C(B41)	0.136(1)	0.293(2)	0.437(1)	8.7(9)
C(A42)	0.681(1)	-0.0208(9)	-0.215(2)	8.7(9)	C(B42)	0.086(2)	0.220(1)	0.376(2)	10(1)
C(A43)	0.699(2)	-0.045(1)	-0.2612(9)	10(1)	C(B43)	0.024(2)	0.246(2)	0.355(2)	18(2)
C(A44)	0.758(2)	-0.0753(9)	-0.242(2)	6.5(7)	C(B44)	0.12(1)	0.287(2)	0.394(1)	13(1)
C(A45)	0.799(1)	-0.0819(9)	-0.176(2)	11(1)	C(B45)	0.062(2)	0.300(1)	0.455(2)	21(2)
C(A46)	0.781(2)	-0.058(1)	-0.1300(9)	8.9(9)	C(B46)	0.124(2)	0.274(2)	0.477(2)	18(2)
C(A51)	0.864(1)	-0.2183(9)	0.167(1)	6.3(7)	C(B51)	0.3301(9)	-0.0263(7)	0.6843(6)	4.1(5)
C(A52)	0.888(1)	0.273(1)	0.1628(8)	9(1)	C(B52)	0.3401(8)	0.0128(5)	0.7344(8)	4.8(6)
C(A53)	0.888(1)	0.3179(8)	0.205(1)	10(1)	C(B53)	0.3378(8)	-0.0069(7)	0.7911(7)	6.9(7)
C(A54)	0.865(1)	0.3071(9)	0.252(1)	7.7(8)	C(B54)	0.3256(9)	-0.0657(7)	0.7978(6)	5.3(7)
C(A55)	0.841(1)	0.2075(8)	0.2562(8)	9.5(9)	C(B55)	0.3156(8)	-0.1048(5)	0.7477(8)	5.0(6)
C(A56)	0.840(1)	0.2075(8)	0.214(1)	7.9(8)	C(B56)	0.3178(8)	-0.0851(7)	0.6909(7)	5.5(6)
C(A61)	0.953(2)	0.169(1)	0.128(1)	7.3(8)	C(B61)	0.392(1)	-0.0412(8)	0.598(2)	5.2(6)
C(A62)	1.006(3)	0.165(1)	0.189(3)	7.3(8)	C(B62)	0.452(2)	-0.0458(8)	0.653(2)	5.1(6)
C(A63)	1.069(2)	0.182(1)	0.197(3)	8.3(9)	C(B63)	0.508(1)	-0.0670(8)	0.6478(7)	6.6(7)
C(A64)	1.079(2)	0.203(1)	0.144(1)	15(2)	C(B64)	0.504(1)	-0.0836(8)	0.588(2)	7.5(7)
C(A65)	1.025(3)	0.207(1)	0.084(3)	18(2)	C(B65)	0.444(2)	-0.0789(8)	0.533(2)	4.7(6)
C(A66)	0.962(2)	0.190(1)	0.076(2)	14(2)	C(B66)	0.388(1)	-0.0577(8)	0.5378(7)	4.8(6)
C(A71)	0.8632(9)	-0.0343(7)	0.1789(8)	4.5(5)	C(B71)	0.2355(9)	-0.0542(7)	0.4222(7)	5.5(6)
C(A72)	0.8945(8)	-0.0841(8)	0.1851(7)	6.4(7)	C(B72)	0.2444(9)	-0.1134(8)	0.4378(7)	5.8(7)
C(A73)	0.8909(9)	-0.1298(6)	0.2279(9)	7.4(8)	C(B73)	0.2656(9)	-0.1511(5)	0.4026(9)	6.6(7)
C(A74)	0.8560(9)	-0.1178(7)	0.2645(8)	6.5(7)	C(B74)	0.2780(9)	-0.1296(7)	0.3518(7)	6.2(7)
C(A75)	0.8246(8)	-0.0640(8)	0.2583(7)	5.5(6)	C(B75)	0.2691(9)	-0.0703(8)	0.3361(7)	6.1(7)
C(A76)	0.8282(9)	-0.0222(6)	0.2155(9)	4.9(6)	C(B76)	0.2478(9)	-0.0326(5)	0.3713(9)	4.3(6)
C(A81)	0.953(2)	0.0071(9)	0.1294(7)	5.1(6)	C(B81)	0.122(1)	-0.0473(4)	0.447(4)	5.9(7)
C(A82)	0.963(3)	-0.0185(9)	0.079(2)	5.6(6)	C(B82)	0.082(4)	-0.035(1)	0.380(5)	10(1)
C(A83)	1.026(2)	-0.0359(8)	0.088(2)	4.9(6)	C(B83)	0.017(3)	-0.053(1)	0.357(2)	13(1)
C(A84)	1.079(2)	-0.0277(9)	0.1482(7)	7.5(8)	C(B84)	-0.009(1)	-0.070(1)	0.401(4)	14(1)
C(A85)	1.069(3)	-0.0021(9)	0.199(2)	7.9(9)	C(B85)	-0.031(4)	-0.069(1)	0.467(5)	21(2)
C(A86)	1.006(2)	0.0153(8)	0.189(2)	6.3(7)	C(B86)	0.097(3)	-0.050(1)	0.490(2)	23(3)



TABLE 36. (Continued)

## Rigid Group Parameters

	<sup>a</sup> Xc	Yc	Zc	<sup>b</sup> Delta	Epsilon	Eta
Ring1	0.6130(5)	0.2526(6)	-0.1568(6)	-0.44(1)	1.57(1)	4.30(1)
Ring2	0.5282(6)	0.0967(5)	-0.0703(6)	1.14(1)	2.89(3)	2.39(3)
Ring3	0.5699(6)	-0.0640(5)	-0.1087(5)	3.84(1)	2.87(1)	3.93(1)
Ring4	0.7400(7)	-0.0513(6)	-0.1956(7)	2.13(1)	2.04(2)	3.98(3)
Ring5	0.8643(6)	0.2627(7)	0.2095(7)	0.28(1)	1.27(1)	5.42(2)
Ring6	1.0157(8)	0.1860(7)	0.1363(9)	4.34(2)	2.64(4)	0.86(5)
Ring7	0.8596(5)	-0.0761(5)	0.2217(5)	2.76(1)	1.11(1)	5.45(1)
Ring8	1.0160(6)	-0.0103(5)	0.1388(6)	2.01(1)	2.76(3)	5.56(3)
Ring9	0.3864(5)	0.2734(5)	0.7205(6)	3.21(1)	1.87(1)	0.57(1)
Ring10	0.4616(6)	0.2392(5)	0.5489(6)	1.33(1)	2.16(5)	4.61(5)
Ring11	0.2576(5)	0.2659(6)	0.3594(6)	3.27(1)	1.35(1)	2.64(1)
Ring12	0.074(1)	0.2600(8)	0.416(1)	-0.83(2)	2.65(3)	3.85(3)
Ring13	0.3278(5)	-0.0460(5)	0.7410(5)	0.19(1)	1.60(1)	0.34(1)
Ring14	0.4481(6)	-0.0624(5)	0.5928(6)	-1.20(1)	2.43(3)	1.26(3)
Ring15	0.2567(5)	-0.0919(5)	0.3870(6)	-0.18(1)	1.31(1)	2.46(1)
Ring16	0.0569(9)	-0.0517(7)	0.424(1)	4.37(2)	2.13(6)	4.25(6)

<sup>a</sup><sup>b</sup> Xc, Yc and Zc are the fractional coordinates of the centroid of the rigid group.

The rigid group orientation angles Delta, Epsilon and Eta (radians) are the angles by which the rigid body is rotated with respect to a set of axes X, Y and Z. The origin is the centre of the ring; X is parallel to a\*, Z is parallel to c and Y is parallel to the line defined by the intersection of the plane containing a\* and b\* with the plane containing b and c.

TABLE 37. Idealized Positional and Thermal Parameters for the Hydrogen Atoms of [Rh<sub>2</sub>C<sub>12</sub>(CO)<sub>2</sub>(C<sub>2</sub>S<sub>4</sub>)(DPM)<sub>2</sub>].

Atom	X	Y	Z	B(A <sup>1</sup> )	Atom	X	Y	Z	B(A <sup>1</sup> )
H(A1)	0.7019	0.0928	-0.1492	5.58	H(A83)	1.0331	-0.0532	0.0542	5.85
H(A2)	0.6293	0.0749	-0.1675	5.58	H(A84)	1.1227	-0.0405	0.1554	8.49
H(A3)	0.8358	0.0931	0.1805	4.85	H(A85)	1.1059	0.0017	0.2407	8.93
H(A4)	0.9122	0.0933	0.2067	4.85	H(A86)	0.9995	0.0312	0.2248	7.31
H(B1)	0.2787	0.2769	0.5269	7.21	H(B12)	0.3804	0.1722	0.7240	6.49
H(B2)	0.2425	0.2441	0.5616	7.21	H(B13)	0.4152	0.2264	0.8199	7.32
H(B3)	0.2153	-0.0281	0.5708	6.45	H(B14)	0.4220	0.3286	0.8168	6.37
H(B4)	0.2527	-0.0751	0.5506	6.45	H(B15)	0.3940	0.3765	0.7179	9.98
H(A12)	0.6519	0.1783	-0.2020	7.61	H(B16)	0.3592	0.3222	0.6220	7.29
H(A13)	0.6073	0.2640	-0.2606	8.80	H(B22)	0.3537	0.2243	0.4661	7.59
H(A14)	0.5685	0.3384	-0.2150	8.46	H(B23)	0.4406	0.2486	0.4389	5.68
H(A15)	0.5742	0.3269	-0.1108	8.60	H(B24)	0.5475	0.2633	0.5206	7.71
H(A16)	0.6187	0.2411	-0.0522	5.64	H(B25)	0.5673	0.2537	0.6295	8.60
H(A22)	0.6277	0.0821	0.0237	6.55	H(B26)	0.4803	0.2293	0.6567	6.11
H(A23)	0.5266	0.0511	0.0211	7.44	H(B32)	0.2449	0.3186	0.4424	6.83
H(A24)	0.4282	0.0651	-0.0723	7.79	H(B33)	0.2749	0.3686	0.3694	8.92
H(A25)	0.4309	0.1103	-0.1633	8.56	H(B34)	0.2873	0.3174	0.2863	7.50
H(A26)	0.5320	0.1413	-0.1608	6.24	H(B35)	0.2697	0.2161	0.2764	7.14
H(A32)	0.5585	0.0137	-0.1800	5.99	H(B36)	0.2397	0.1660	0.3494	6.96
H(A39)	0.4660	-0.0429	-0.1937	5.99	H(B42)	0.0958	0.1907	0.3523	11.30
H(A34)	0.4769	-0.1207	-0.1230	6.64	H(B43)	-0.0092	0.2339	0.3147	19.15
H(A35)	0.5804	-0.1419	-0.0387	6.28	H(B44)	-0.0316	0.3028	0.3787	14.26
H(A36)	0.6729	-0.0852	-0.0249	6.07	H(B45)	0.0510	0.3285	0.4804	21.90
H(A42)	0.6406	0.0001	-0.2308	9.67	H(B46)	0.1560	0.2853	0.5180	19.20
H(A43)	0.6720	-0.0437	-0.3062	10.88	H(B52)	0.3476	0.0522	0.7308	5.81
H(A44)	0.7712	-0.0965	-0.2707	7.46	H(B53)	0.3456	0.0182	0.8267	7.92
H(A45)	0.8391	-0.1054	-0.1597	11.56	H(B54)	0.3259	-0.0810	0.8378	6.95
H(A46)	0.8077	-0.0616	-0.0843	9.86	H(B55)	0.3082	-0.1462	0.7528	5.99
H(A52)	0.9015	0.2779	-0.1291	9.86	H(B56)	0.3101	-0.1123	0.6568	6.51
H(A54)	0.8656	0.3543	0.1981	11.26	H(B62)	0.4521	-0.0341	0.6927	6.12
H(A55)	0.8264	0.2457	0.2782	8.69	H(B63)	0.5467	-0.0705	0.6851	7.61
H(A56)	0.8247	0.1693	0.2893	10.54	H(B64)	0.5411	-0.0993	0.5844	8.54
H(A62)	0.9977	0.1492	0.2202	8.86	H(B65)	0.4410	-0.0917	0.4915	5.68
H(A63)	1.1032	0.1796	0.2253	8.28	H(B66)	0.3465	-0.0554	0.4991	5.80
H(A65)	1.1198	0.2135	0.2393	9.27	H(B72)	0.2379	-0.1269	0.4732	6.78
H(A66)	1.0308	0.2169	0.1504	15.99	H(B73)	0.2741	-0.1905	0.4145	7.62
H(A72)	0.9254	0.1864	0.0476	18.62	H(B74)	0.2940	-0.1547	0.3283	7.22
H(A73)	0.9146	0.0969	0.0336	15.41	H(B75)	0.2776	-0.0553	0.3008	7.15
H(A74)	0.9093	-0.1677	0.1560	7.45	H(B76)	0.2414	0.0083	0.3595	5.33
H(A75)	0.8540	-0.1470	0.2278	8.40	H(B82)	0.0953	-0.0238	0.3476	10.51
H(A76)	0.8040	-0.0555	0.2926	7.49	H(B83)	-0.0132	-0.0583	0.3137	14.36
H(A77)	0.8093	0.0153	0.2855	6.46	H(B84)	-0.0509	-0.0877	0.3905	14.65
H(A82)	0.9267	-0.0237	0.2136	5.92	H(B85)	0.0199	-0.0826	0.5011	21.72
			0.0382	6.55	H(B86)	0.1284	-0.0481	0.5349	24.40

Table 38. Least Squares Plane Calculations

Plane No.	Dimer	Equation <sup>a</sup>
1	A	0.8729X+0.1141Y-0.4743Z-14.9811 = 0.0
	B	0.8952X-0.0956Y-0.4353Z+4.0804 = 0.0
2	A	0.8862X+0.0856Y-0.4553Z-15.1615 = 0.0
	B	0.8948X-0.1440Y-0.4227Z+4.0503 = 0.0
3	A	-0.6211X-0.0716Y-0.7804Z+11.0834 = 0.0
	B	0.0947X+0.9925Y-0.0779Z-1.4659 = 0.0

deviation from planes, Å						
Plane no.						
Atom	1-A	1-B	2-A	2-B	3-A	3-B
Rh(1)	0.027(2)	-0.010(2)	-0.012(2)	0.002(2)	-0.015(2)	0.010(2)
Rh(2)	-0.030(2)	0.012(2)	0.013(2)	-0.003(2)	0.033(2)	-0.007(2)
P(1)	-0.326(8)	0.121(8)				
P(2)	0.312(8)	-0.143(9)				
P(3)			0.163(8)	-0.027(8)		
P(4)			-0.154(8)	0.030(8)		
S(1)					-0.110(7)	-0.065(7)
S(2)					0.26(1)	0.012(9)
S(3)					0.141(8)	-0.018(7)
S(4)					-0.355(7)	0.035(7)
C(2)	0.67(3) <sup>b</sup>	-0.63(3) <sup>b</sup>				
C(3)			-0.74(3) <sup>b</sup>	-0.54(3)		
C(4)					0.14(3)	-0.03(3)
C(5)					-0.11(3)	0.01(2)

<sup>a</sup>X, Y, and Z are orthogonal coordinates (Å) with X along the a axis, Y in the a-b plane and Z along the c\* axis.

<sup>b</sup>Not included in least-squares plane calculations.

Table 39: Select Distances (Å) in  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$ 

	Bond Distance	
	Dimer A	Dimer B
Rh(1) - Rh(2)	2.810 (3)	2.809 (3)
Rh(1) - Cl(1)	2.427 (6)	2.454 (6)
Rh(2) - Cl(2)	2.507 (8)	2.529 (8)
Rh(1) - P(1)	2.353 (7)	2.326 (7)
Rh(2) - P(2)	2.359 (7)	2.345 (8)
Rh(1) - P(3)	2.367 (8)	2.349 (7)
Rh(2) - P(4)	2.346 (8)	2.371 (7)
Rh(1) - S(1)	2.351 (7)	2.356 (7)
Rh(1) - C(5)	1.89 (2)	1.95 (2)
Rh(2) - S(4)	2.388 (7)	2.392 (7)
Rh(2) - C(1)	1.86 (2)	1.97 (3)
S(1) - C(4)	1.67 (2)	1.73 (2)
S(2) - C(4)	1.62 (3)	1.64 (3)
S(3) - C(4)	1.79 (2)	1.73 (3)
S(3) - C(5)	1.76 (2)	1.74 (2)
S(4) - C(5)	1.68 (3)	1.63 (2)
C(1) - O(1)	1.13 (2)	1.01 (3)
P(1) - C(2)	1.85 (2)	1.86 (2)
P(2) - C(2)	1.84 (2)	1.86 (2)
P(3) - C(3)	1.85 (2)	1.78 (3)
P(4) - C(3)	1.84 (2)	1.88 (3)
P(1) - C(11)	1.84 (1)	1.82 (1)
P(1) - C(21)	1.85 (1)	1.83 (1)
P(2) - C(31)	1.84 (1)	1.80 (1)
P(2) - C(41)	1.86 (1)	1.86 (2)
P(3) - C(51)	1.89 (2)	1.84 (1)
P(3) - C(61)	1.86 (2)	1.84 (1)
P(4) - C(71)	1.85 (1)	1.82 (1)
P(4) - C(81)	1.85 (1)	1.84 (2)

## Nonbonded Contacts

P(A1) - P(A2)	3.018 (9)
P(B1) - P(B2)	3.088 (10)
P(A3) - P(A4)	3.022 (10)
P(B3) - P(B4)	3.096 (10)
Cl(A2) - H(A46)	2.39
Cl(B2) - H(B42)	2.58
O(A1) - H(A22)	2.48
C(B3) - H(B22)	2.33
H(A76) - H(A3)	2.11
H(A86) - H(A4)	2.30
H(A13) - H(B25) <sup>a</sup>	2.29
H(A65) - H(B45) <sup>b</sup>	2.05

<sup>a</sup> Atom located at  $x, y, -1+z$ .<sup>b</sup> Atom located at  $1+x, 1-y, -1+z$ .

Table 40. Selected Angles (deg) in  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$ Bond Angles

	Dimer A	Dimer B
Rh(2)-Rh(1)-S(1)	163.0(2)	164.4(2)
Rh(2)-Rh(1)-Cl(1)	104.1(2)	91.7(2)
Rh(2)-Rh(1)-C(5)	74.7(8)	76.3(7)
Rh(2)-Rh(1)-P(1)	88.9(2)	95.3(2)
Rh(2)-Rh(1)-P(3)	93.5(2)	92.3(2)
Rh(1)-Rh(2)-Cl(2)	172.9(2)	165.5(2)
Rh(1)-Rh(2)-S(4)	72.6(2)	71.5(2)
Rh(1)-Rh(2)-C(1)	91.9(8)	100.4(8)
Rh(1)-Rh(2)-P(2)	94.2(2)	91.2(2)
Rh(1)-Rh(2)-P(4)	91.2(2)	94.7(2)
Cl(1)-Rh(1)-S(1)	92.9(2)	103.8(2)
Cl(1)-Rh(1)-C(5)	177.5(8)	166.9(7)
Cl(1)-Rh(1)-P(1)	91.0(2)	86.6(2)
Cl(1)-Rh(1)-P(3)	83.0(2)	93.0(2)
Cl(2)-Rh(2)-S(4)	101.2(2)	94.0(2)
Cl(2)-Rh(2)-C(1)	94.4(8)	94.1(8)
Cl(2)-Rh(2)-P(2)	88.2(2)	89.2(3)
Cl(2)-Rh(2)-P(4)	86.1(3)	86.5(3)
S(1)-Rh(1)-C(5)	88.3(8)	88.3(7)
S(1)-Rh(1)-P(1)	92.0(2)	86.5(3)
S(1)-Rh(1)-P(3)	87.4(2)	86.3(2)
S(4)-Rh(2)-C(1)	164.3(8)	171.8(8)
S(4)-Rh(2)-P(2)	82.4(2)	94.4(2)
S(4)-Rh(2)-P(4)	96.3(2)	93.0(2)
C(5)-Rh(1)-P(1)	91.2(8)	89.3(7)
C(5)-Rh(1)-P(3)	94.8(8)	92.8(7)
C(1)-Rh(2)-P(2)	96.4(8)	87.2(8)
C(1)-Rh(2)-P(4)	86.4(8)	86.0(8)
P(1)-Rh(1)-P(3)	173.9(2)	172.4(3)
P(2)-Rh(2)-P(4)	173.8(2)	171.7(3)
Rh(1)-S(1)-C(4)	105.1(9)	104.5(9)
S(1)-C(4)-S(2)	127(2)	123(1)
S(1)-C(4)-S(3)	118(1)	119(2)
S(2)-C(4)-S(3)	115(1)	117(1)
C(4)-S(3)-C(5)	102(1)	104(1)
Rh(1)-C(5)-S(3)	124(1)	124(1)
Rh(1)-C(5)-S(4)	120(1)	117(1)
S(3)-C(5)-S(4)	116(1)	119(1)
Rh(2)-S(4)-C(5)	91.1(8)	95.1(8)
Rh(2)-C(1)-O(1)	169(3)	165(3)

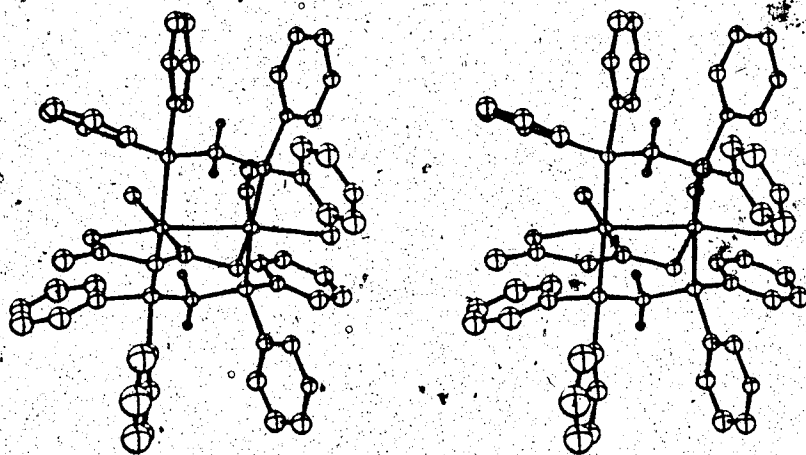
Table 40, continued

<u>Bond Angles</u>		
	Dimer A	Dimer B
Rh(1)-P(1)-C(2)	114.4(8)	110.7(9)
Rh(2)-P(2)-C(2)	113.2(8)	116(1)
Rh(1)-P(3)-C(3)	108.5(8)	115.4(9)
Rh(2)-P(4)-C(3)	114.7(8)	110.7(8)
Rh(1)-P(1)-C(11)	115.3(6)	117.2(7)
Rh(1)-P(1)-C(21)	126.1(6)	116.7(6)
Rh(2)-P(2)-C(31)	117.1(6)	121.9(9)
Rh(2)-P(2)-C(41)	118.8(8)	116(1)
Rh(1)-P(3)-C(51)	113.5(7)	117.8(6)
Rh(1)-P(3)-C(61)	128(1)	112.8(6)
Rh(2)-P(4)-C(71)	115.5(6)	120.0(6)
Rh(2)-P(4)-C(81)	116.9(7)	116.6(8)
P(1)-C(2)-P(2)	110(1)	112(1)
P(3)-C(3)-P(4)	110(1)	115(1)
C(2)-P(1)-C(11)	102(1)	100(1)
C(2)-P(1)-C(21)	99.1(9)	110(1)
C(2)-P(2)-C(31)	105.8(9)	102(1)
C(2)-P(2)-C(41)	101(1)	99(1)
C(3)-P(3)-C(51)	105(1)	99(1)
C(3)-P(3)-C(61)	104(1)	108(1)
C(3)-P(4)-C(71)	100.9(9)	105(1)
C(3)-P(4)-C(81)	106(1)	99(1)
C(11)-P(1)-C(21)	99.1(8)	101.4(8)
C(31)-P(2)-C(41)	99.1(8)	97(1)
C(51)-P(3)-C(61)	94(1)	102.4(8)
C(71)-P(4)-C(81)	100.5(9)	102(1)

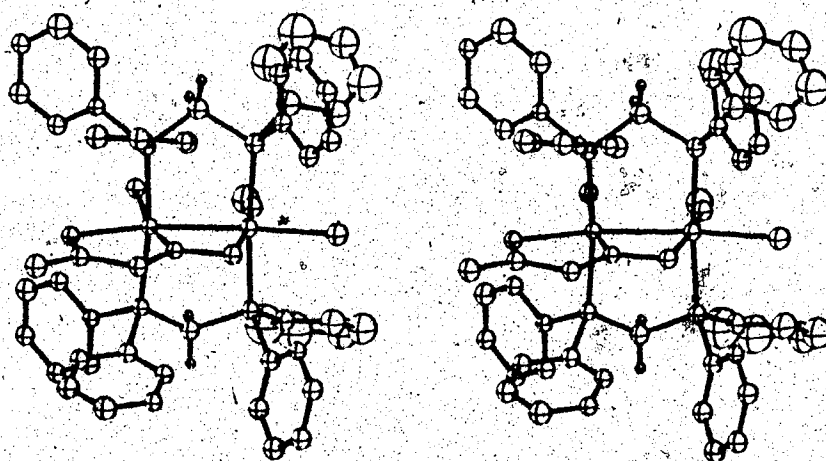
<u>Torsion Angles</u>		
	Dimer A	Dimer B
P(1)-Rh(1)-Rh(2)-P(2)	17.0(2)	7.1(2)
P(3)-Rh(1)-Rh(2)-P(4)	8.4(2)	1.5(2)
C(11)-Rh(1)-P(1)-C(11)	98.8(7)	49.5(7)
C(11)-Rh(1)-P(1)-C(21)	25.5(8)	170.0(7)
C(11)-Rh(1)-P(3)-C(51)	45.6(8)	42.4(7)
C(11)-Rh(1)-P(3)-C(61)	162(1)	161.4(7)
C(11)-Rh(2)-P(2)-C(31)	70.1(6)	54.4(8)
C(11)-Rh(2)-P(2)-C(41)	48.9(7)	64(1)
C(11)-Rh(2)-P(4)-C(71)	51.9(7)	62.0(8)
C(11)-Rh(2)-P(4)-C(81)	66.0(7)	62(1)
S(1)-Rh(1)-P(1)-C(11)	5.9(7)	54.6(7)
S(1)-Rh(1)-P(1)-C(21)	118.4(7)	65.9(7)
S(1)-Rh(1)-P(3)-C(51)	47.6(8)	61.3(7)

Table 40, continued

<u>Torsion Angles</u>		
	Dimer A	Dimer B
S(1)-Rh(1)-P(3)-C(61)	69 (1)	57.7(7)
S(4)-Rh(2)-P(2)-C(31)	171.6(6)	39.6(8)
S(4)-Rh(2)-P(2)-C(41)	52.7(7)	158 (1)
S(4)-Rh(2)-P(4)-C(71)	152.8(7)	31.8(8)
S(4)-Rh(2)-P(4)-C(81)	34.9(7)	156 (1)
C(5)-Rh(1)-P(1)-C(11)	82 (1)	142.9(9)
C(5)-Rh(1)-P(1)-C(21)	153 (1)	22 (1)
C(5)-Rh(1)-P(3)-C(51)	136 (1)	149.4(9)
C(5)-Rh(1)-P(3)-C(61)	19 (1)	30 (1)
C(1)-Rh(2)-P(2)-C(31)	24 (1)	148 (1)
C(1)-Rh(2)-C(41)	143 (1)	30 (1)
C(1)-Rh(2)-P(4)-C(71)	143 (1)	156 (1)
C(1)-Rh(2)-P(4)-C(81)	161 (1)	32 (1)



(A)



(B)

Figure 22. Stereoviews for Molecules A and B of  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$ .





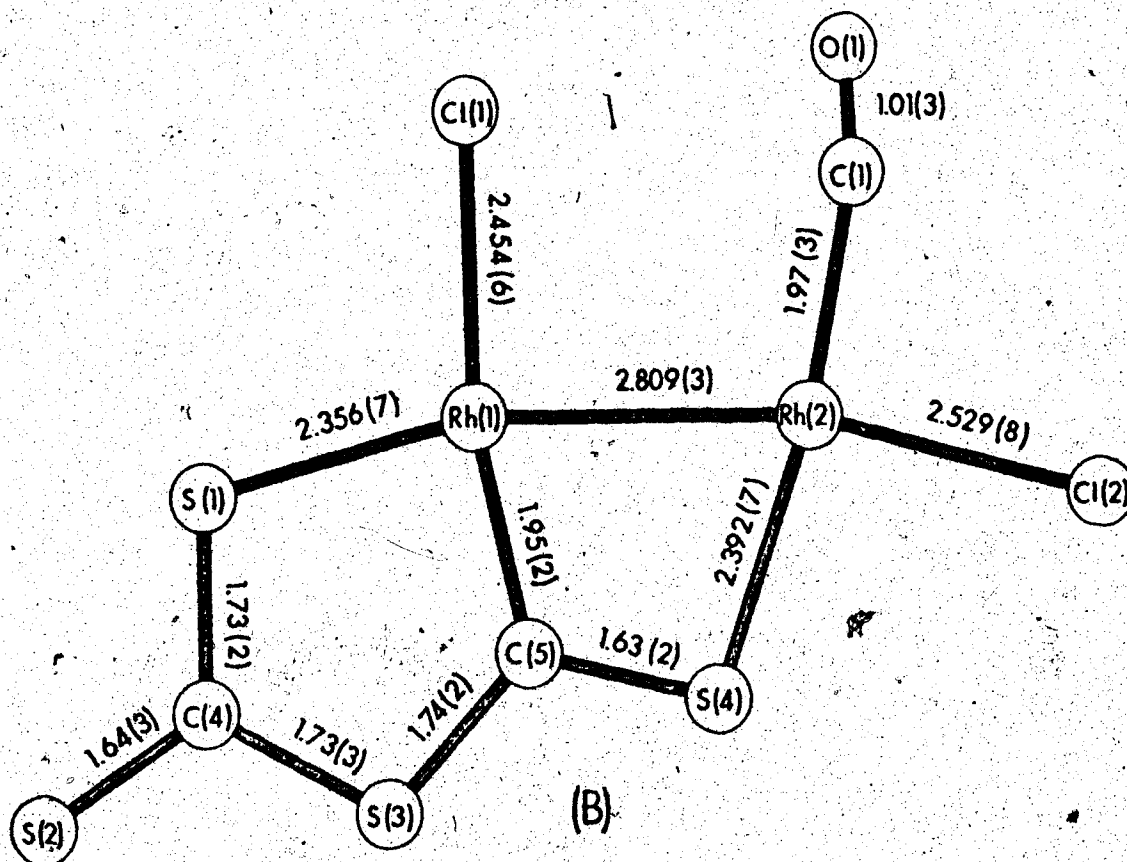
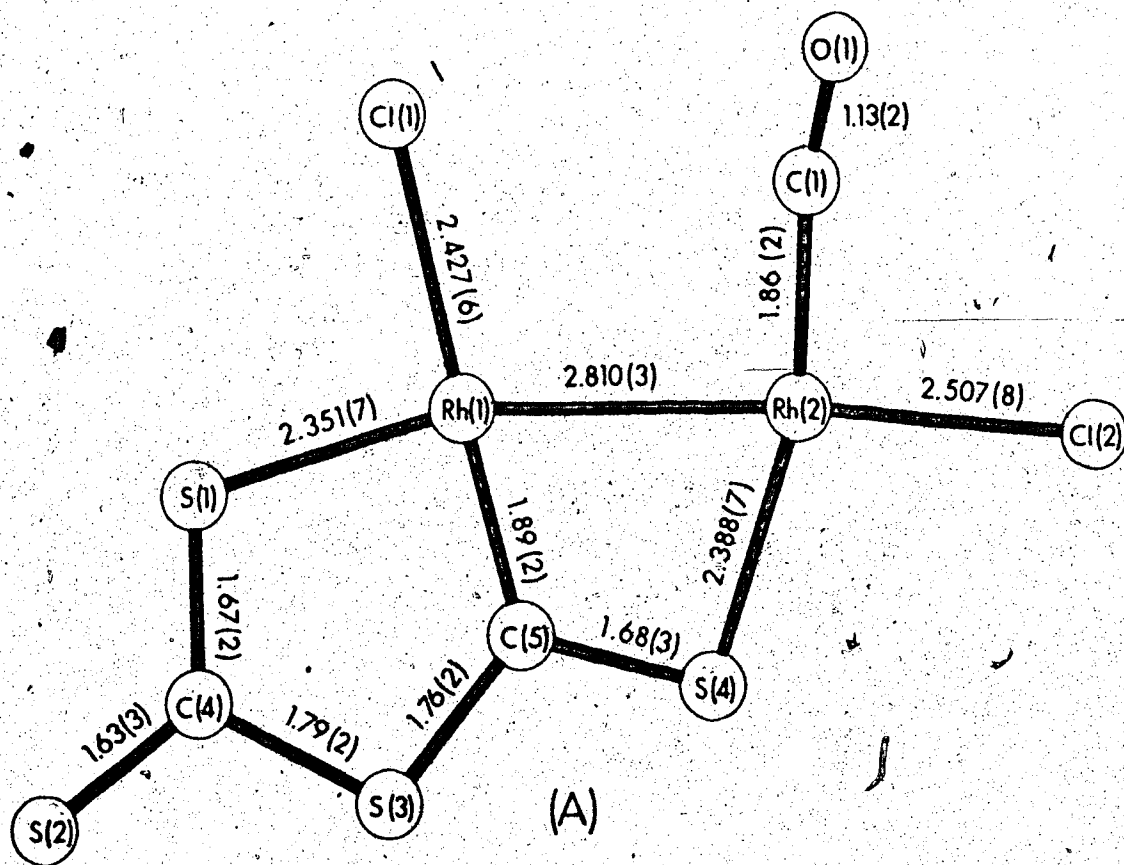


Figure 24. The Equatorial Planes of Dimers A and B of  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$ .

## DISCUSSION

### Description of Structure

The complex,  $[\text{Rh}_2\text{Cl}_2(\text{CO})(\text{C}_2\text{S}_4)(\text{DPM})_2]$  (3), crystallizes with two independent molecules per asymmetric unit. Both dimers have the same overall geometry, with the Rh centres bridged by two transoid DPM ligands, but differ slightly in the orientations of the ligands (vide infra). Within each dimer the Rh atoms display distorted octahedral coordinations. One rhodium atom of each dimer (Rh(A1), Rh(B1)) has two mutually trans P atoms in the axial sites with the equatorial positions occupied by a sulfur and a carbon atom of the  $\text{C}_2\text{S}_4$  fragment, a chloro ligand and the other Rh atom. The second Rh atom (Rh(A2), Rh(B2)) also has mutually trans axial P atoms, with a sulfur atom of the  $\text{C}_2\text{S}_4$  moiety, a chloro ligand, a carbonyl ligand and the other Rh atom occupying its equatorial sites.

The Rh-Rh distances of  $2.810(3)\text{\AA}$  and  $2.809(3)\text{\AA}$ , for dimers A and B, respectively, compare well with each other and are consistent with a normal Rh-Rh single bond, falling within the range previously reported for such distances ( $2.617(3)$  to  $2.8415(7)\text{\AA}$ ).<sup>129-133</sup>

The Rh-C and C-O distances of the carbonyl ligands are not unusual, comparing acceptably with other determinations.<sup>35,120,126</sup> However, both carbonyl groups are significantly bent ( $\text{Rh(A2)-C(A1)-O(A1)} = 169(3)^\circ$ ,  $\text{Rh(B2)-C(B1)-O(B1)} = 165(3)^\circ$ ). A consideration of the nonbonded contacts indi-

cates that in both dimers the carbonyl ligands bend in such a way as to minimize the contacts with the phenyl rings suggesting that the bending of these ligands is steric in origin.

The rhodium-chlorine distances ( $\text{Rh(A1)-Cl(A1)} = 2.427(6)\text{\AA}$ ;  $\text{Rh(B1)-Cl(B1)} = 2.454(6)\text{\AA}$ ) which are trans to C(A5) and C(B5), respectively, are quite long but compare well with other determinations, where the chloro ligand is trans to a  $\sigma$ -bound alkyl group or carbene ligand.<sup>163-165</sup> On the other hand, the Rh(2)-Cl(2) bond distances ( $2.507(8)\text{\AA}$  and  $2.529(8)\text{\AA}$  for molecules A and B, respectively), which are opposite the rhodium atoms, Rh(A1) and Rh(B1), are significantly longer than those typically observed in these systems;<sup>96,125,126</sup> in fact they are even longer than those observed when a chloro ligand is opposite a ligand of high trans influence such as a carbene. These long rhodium-chloro distances probably arise as a result of steric crowding about the Rh(2) centre. Support for this comes from the short nonbonded phenyl hydrogen-chloro contacts observed for these two chloro ligands ( $\text{Cl(A2)-H(A46)} = 2.39\text{\AA}$ ;  $\text{Cl(B2)-H(B42)} = 2.58\text{\AA}$ ). Further, these interactions are such that they tend to force these chloro ligands away from the metal centres (see Figures 22 and 23).

The  $\text{C}_2\text{S}_4$  fragment contains two intact  $\text{CS}_2$  molecules ( $\text{S(1)C(4)S(2)}$  and  $\text{S(3)C(5)S(4)}$ ) fused at  $\text{C(4)-S(3)}$ . This fragment is then bound to one rhodium atom (Rh(1)) via S(1) and C(5) and to the other rhodium atom through S(4).

Within the resulting  $\text{Rh}_2\text{C}_2\text{S}_4$  metallocycles the C-S distances (1.63(2)-1.79(2) Å) and angles (see Table 40) compare favourably with those reported for  $[\text{Rh}(\eta^5\text{-C}_5\text{H}_5)(\text{C}_2\text{S}_4)(\text{PMe}_3)]$ ,<sup>162</sup> where an analogous  $\text{C}_2\text{S}_4$  fragment was observed. These distances suggest delocalization over the carbon-sulfur framework and range from values comparable to the C-S double bond distance observed in ethylene thiourea (1.71 Å)<sup>166</sup> to single bond values (1.81 Å).<sup>166</sup> The Rh(1)-S(1) and Rh(2)-S(4) distances (average 2.354(7) Å and 2.390(7) Å, respectively), although significantly different compare favourably with other determinations.<sup>163,164,167,168</sup>

The  $\text{C}_2\text{S}_4$  ligand can be considered as a carbene ligand,  $\text{C}_2\text{S}_4^{2-}$ , with each of the coordinated sulfur atoms functioning as a two electron donor to the rhodium atoms, leaving the carbene carbon atom as a two electron donor. Therefore the rhodium atoms are formally Rh(II). The unusually short Rh(1)-C(5) distances (1.89(2) and 1.95(2), for dimers A and B respectively) are comparable to the rhodium carbonyl distances indicating significant multiple bond character. These rhodium-carbene distances are comparable to other such distances and are especially close to those observed in  $[\text{RhCl}(\text{PPh}_3)_2(\text{PhCONCS})_2]$ <sup>163</sup> and  $[\text{RhCl}(\text{PPh}_3)_2(\text{EtOCONCS})_3]$ .<sup>164</sup> In these complexes five membered metallocycle rings again resulted as a consequence of condensation of sulfur-containing molecules on rhodium.

Within the DPM framework the parameters are, on the whole, not unusual and compare well with other determin-

ations. 35, 89, 96, 120, 126 The P-C-C angles, for example, (range 125(2) to 115(2)°) do not deviate significantly from the expected value of 120° and compare favourably with other similar compounds. However it is significant that the methylene orientations in the two dimers are different. In dimer A a trans methylene arrangement is observed whereas these groups are cis in dimer B. Based on previous work it was anticipated that the methylene groups of the DPM ligands would fold in a cis manner towards the  $C_2S_4$  fragment (i.e. towards the site of the bulkier ligand). In dimer B, where the expected cis methylene arrangement is observed the phenyl rings avoid unusually short contacts with the  $C_2S_4$  fragment and as a result this fragment is quite planar. Here, phenyl rings 2 and 6 are parallel to the  $C_2S_4$  moiety, instead of perpendicular to it as is typically observed for the endo phenyl groups of cis oriented methylene groups. This phenyl ring orientation minimizes interactions with the  $C_2S_4$  moiety but tends to force the two other endo phenyl rings 3 and 7 away from their normal orientation (see Chapter VI, for example). However, in dimer A the trans methylene arrangement thrusts ring 6 close to the  $C_2S_4$  fragment resulting in a significant puckering of this fragment (see Figure 22 and Table 38). Therefore, despite comparable bond angle and distance within the  $Rh_2C_2S_4$  metallocycles, significant differences in their overall geometries are present as a result of these phenyl ring interactions.

The differences noted above between the phenyl ring orientations in dimers A and B also lead to differences in the equatorial chloro and carbonyl ligands (see Figure 24) with these ligands tending to stagger themselves with respect to the phenyl rings (see Torsion Angles, Table 40) to again minimize nonbonded contacts. This staggering of the phenyl rings with respect to the equatorial ligands is further assisted in dimer A by a skewing of the Rh-P framework. Without this skewing of the Rh-P framework the phenyl rings of P(A2) would be essentially eclipsed with the chloro and carbonyl ligands of Rh(A2). Whereas, in dimer B because of the *cis* methylene orientation and the subsequent phenyl group orientations no skewing is necessary to maintain normal nonbonded contacts. Therefore, most differences observed between the two dimers are a direct result of the differing methylene orientations.

Reaction of *trans*-[RhCl(CO)(DPM)]<sub>2</sub> and [Rh<sub>2</sub>Cl<sub>2</sub>( $\mu$ -CO)-(DPM)<sub>2</sub>] with CS<sub>2</sub>

The reaction of either *trans*-[RhCl(CO)(DPM)]<sub>2</sub> (1) or [Rh<sub>2</sub>Cl<sub>2</sub>( $\mu$ -CO)(DPM)<sub>2</sub>] with CS<sub>2</sub> results in the isolation of the final product, [Rh<sub>2</sub>Cl<sub>2</sub>(CO)(C<sub>2</sub>S<sub>4</sub>)(DPM)<sub>2</sub>] (3). Based on analogies with the previous studies involving SO<sub>2</sub><sup>96</sup> (Chapters IV and V) and acetylene<sup>42</sup> molecules we can postulate a scheme for the reaction of 1 with CS<sub>2</sub>. Initial attack is probably terminal, since this is the only site open (see Chapter III). The resulting species [Rh<sub>2</sub>Cl(CO)-(CS<sub>2</sub>)( $\mu$ -Cl)( $\mu$ -CO)(DPM)<sub>2</sub>] (4), (see Figure 25) although not

observed is analogous to that proposed for  $\text{SO}_2$  (Chapter IV). This species we believe then rearranges to  $[\text{Rh}_2(\text{CO})_2^-(\mu\text{-Cl})(\mu\text{-CS}_2)(\text{DPM})_2][\text{Cl}]$  (5), which is a 1:1 electrolyte in acetone and dichloromethane, and has a very similar infrared spectrum ( $\nu(\text{CO}) = 1990 \text{ cm}^{-1}$ , the  $\text{CS}_2$  region is obscured by bands due to the DPM ligands) and similar  $^{31}\text{P}\{^1\text{H}\}$  NMR spectral parameters ( $\delta = 14.3 \text{ ppm}$ ;  $|\overset{1}{J}_{\text{Rh-P}} + \overset{x}{J}_{\text{Rh-P}}| = 98.2 \text{ Hz}$ )<sup>101</sup> to the well characterized  $\text{SO}_2$  analogue<sup>96</sup> (Chapter IV). Chloride recoordination, loss of one carbonyl ligand and a facile rearrangement would then yield  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\mu\text{-CS}_2)(\text{DPM})_2]$  (6), which although not observed is exactly analogous to an acetylene complex,<sup>42</sup> which has been prepared in our laboratory by the same route and structurally characterized. Electrophilic attack at S(3) of the bound  $\text{CS}_2$  molecule (see Figure 24) by a second  $\text{CS}_2$  molecule would then readily yield the final product 3.

Since the monocarbonyl species 2 is soluble, its reaction during the stepwise addition of  $\text{CS}_2$  was carefully monitored by infrared,  $^{31}\text{P}\{^1\text{H}\}$  and  $^{13}\text{C}\{^{31}\text{P}\{^1\text{H}\}\}$  NMR spectroscopy. For the  $^{13}\text{C}$  NMR experiment  $^{13}\text{CO}$  enriched  $[\text{Rh}_2\text{Cl}_2(\mu\text{-}^{13}\text{CO})(\text{DPM})_2]$  was used. Initially in the  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum resonances assignable to unreacted 2 and two other symmetric species are observed. One resonance can be assigned to compound 5 which was previously characterized and the other is believed to be due to  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CS}_2)(\text{DPM})_2]$  (7) ( $\delta = 15.7 \text{ ppm}$ ;  $|\overset{1}{J}_{\text{Rh-P}} = \overset{x}{J}_{\text{Rh-P}}| = 116.5 \text{ Hz}$ ) (vide supra).



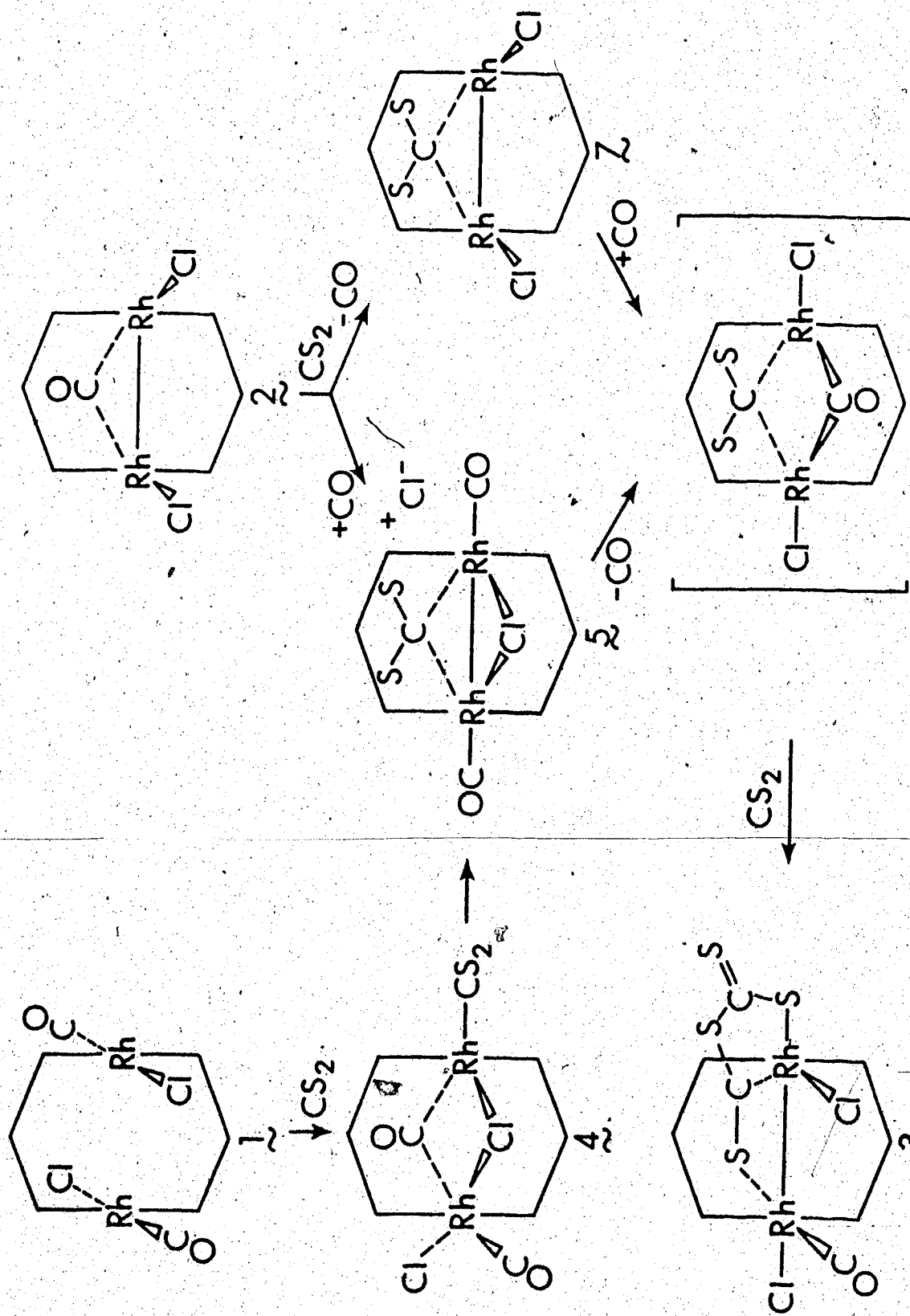


Figure 25. Proposed scheme for the reactions of trans-[RhCl(CO)(DPM)]<sub>2</sub> and [RhCl<sub>2</sub>(μ-CO)(DPM)<sub>2</sub>] with CS<sub>2</sub>.

These observations are consistent with species 5 and 7, shown in Figure 25, resulting from CS<sub>2</sub> attack on 2 and CO transfer. Analogous species have been observed in the reaction of 2 with SO<sub>2</sub> (Chapter V). In these SO<sub>2</sub> studies we observed that these Rh dimers act as efficient CO scavengers. Therefore when 5 loses CO yielding 6, compound 7 picks up CO also giving 6, which subsequently yields the final product 3 by condensation of the second CS<sub>2</sub> molecule (vide supra). Complex 3 shows a complex multiplet ( $\delta = 7.5$  ppm) pattern in the <sup>31</sup>P{<sup>1</sup>H} NMR spectrum, arising from its AA'BB'XY spin system. No resonance assignable to 6 was observed.

Since in compounds 5 and 7 the four phosphorus atoms are equivalent at -50°C, it is suggested that the CS<sub>2</sub> ligand in species 5, 6 and 7 is coordinated solely through the carbon atom, as has been proposed for CO<sub>2</sub> in some of its compounds.<sup>51</sup> A C-S bound species would give rise to a more complex <sup>31</sup>P NMR owing to the resulting chemical inequivalence of the phosphorus atoms unless the CS<sub>2</sub> molecule were fluxional at this temperature. No evidence suggesting fluxionality of these species was observed.

The <sup>13</sup>C NMR spectra of the same reaction initially shows the resonance assignable to 2, as well as one additional species at  $\delta = 186.5$  ppm (doublet,  $|^1J_{\text{Rh-C}}| = 80.1$  Hz), characteristic of a terminal carbonyl ligand and consistent with species 5. The only other carbonyl resonance observed

later in the experiment is assignable to species 3 at  $\delta = 191.5$  ppm (doublet,  $|J_{\text{Rh-C}}| = 69.1$  Hz). Similarly the infrared spectrum shows only bands assignable to 2, 3 and a band at  $1990 \text{ cm}^{-1}$  which is again consistent with species 5. Therefore, all the spectral parameters and the analogies to the  $\text{SO}_2$ <sup>96</sup> and acetylene<sup>42</sup> chemistry appear to support this scheme.

### CONCLUSIONS

This study presents only the second structural characterization<sup>162</sup> of a rhodium-carbon disulfide complex and is the first such binuclear species. Based on its infrared spectrum, which is similar to other Rh-CS<sub>2</sub> complexes, which are believed to contain C,S- $\eta^2$  side-on bound CS<sub>2</sub>, this work suggests that these compounds should probably be reformulated as C<sub>2</sub>S<sub>4</sub> species. Certainly it is becoming apparent that rhodium has a marked tendency for activating and condensing sulfur containing molecules as has now been demonstrated by several structural determinations.<sup>162-164</sup> The similarities in the mode of CS<sub>2</sub> condensation to that of CO<sub>2</sub> in an iridium complex,  $[\text{IrCl}(\text{C}_2\text{O}_4)(\text{PPh}_3)_3]$ ,<sup>50</sup> supports the argument that CS<sub>2</sub> is a useful model for studying CO<sub>2</sub> binding in metal complexes and suggests the possibility of analogous CO<sub>2</sub> binuclear chemistry.

## CHAPTER VIII.

### Summary and Conclusions

One reason for undertaking the present study was to obtain a better understanding of the coordination and activation of CO, CS<sub>2</sub>, and SO<sub>2</sub> utilizing binuclear diphosphine and diarsine bridged complexes. Additionally, the effect of metal proximity on the chemistries of these small molecules was of interest, as well as the potential relevance of such studies to homogeneous catalysis. Although, not all these goals were met, this study was successful in extending our understanding of the chemistry of this class of binuclear complexes.

With regard to the effect of metal proximity on the chemistry of these dirhodium species, one obvious difference, compared to the analogous mononuclear species, is the possibility of bridging coordination modes for these small molecules. This possibility was realized in almost every study, and in fact, the small molecules of interest show a remarkable tendency to finally reside in the bridging site. It is believed that this site is favoured for these Lewis acids since here they are able to accept electron density from both low valent metals. Another related consequence of the metal proximity is the facile ligand rearrangements which occur in these dirhodium complexes. In almost all cases these rearrangements are preceded by halide dissociation and result in a symmetrical arrangement of the

ligands with the better  $\pi$ -acceptor ligand coordinated in the bridging site. The few exceptions, where a symmetric species does not result, are believed to favour their observed geometries as a consequence of the high steric bulk of the ligands involved, as for example in  $[\text{Rh}_2\text{I}(\text{CO})(\mu\text{-CO})(\text{DPM})_2][\text{I}]$  (1) where the large iodo ligands are not both readily coordinated in the same compound.

The site of attack by small molecules in these species is not altogether straight forward. In *trans*- $[\text{RhCl}(\text{CO})(\text{DPM})]_2$  (2), there is probably only one site of attack at the open fifth coordination site on one of the metal centres opposite the second metal atom. However, in the "A-frame" type species attack can be either at the bridging site or at the terminal site, remote from the bridging site. In  $[\text{Rh}_2(\text{CO})_2(\mu\text{-Cl})(\text{DPM})_2]^+$  (3), we (Chapter IV) and others have shown,<sup>35a,91</sup> that  $\text{SO}_2$  attacks the bridging site, whereas CO attacks terminally. In the distorted "A-frame" species  $[\text{Rh}_2\text{Cl}_2(\mu\text{-SO}_2)(\text{DPM})_2]$  (4) and  $[\text{Rh}_2\text{Br}_2(\mu\text{-CO})(\text{DPM})_2]$  (5) we have observed that the bridging site is blocked in the solid state by four phenyl groups. Consistent with this, much of our chemistry indicates terminal attack. However, this is certainly not unambiguous and recent work with acetylenes seems to indicate that direct attack and insertion of the acetylenes into the Rh-Rh bond occurs.<sup>169</sup> The above  $\text{SO}_2$  (4) and monocarbonyl (5) complexes are significantly different from the dicarbonyl "A-frame" species 3 however in that they have a metal-metal bond, which may serve

as a site of attack for the Lewis acids. The reactivity of the metal-metal bond in these systems is shown by the facile reaction of  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\text{DPM})_2]$  (6) with  $\text{CS}_2$ , whereas the dicarbonyl "A-frame" species 3 shows no reaction. Corroborating this finding, other work in our group has shown that the metal-metal bond species 1, 5 and 6 react instantly with acetylenes, whereas species such as 3, in which no metal bond is present, do not react.<sup>169</sup>

Other aspects of the study regarding the activation of the small molecules and the relevance of these studies to catalysis are still in their infancy. In the carbonyl and sulfur dioxide complexes, these small molecules were certainly activated in the molecular orbital and spectroscopic sense (i.e. we noted a large drop in bond order due to a redistribution of electron density in these molecules). However these small molecules were not activated in a catalytic sense, at least not in the very limited context in which we observed them. The two species which had, spectroscopically, the largest activation of CO and  $\text{SO}_2$  were 6 and 4, respectively. In the first species the carbonyl ligand behaved quite normally and attempts to oxidize the coordinated  $\text{SO}_2$  ligand to  $\text{SO}_4^{2-}$  under mildly forcing conditions were unsuccessful. In contrast the  $\text{CS}_2$  molecule is readily activated and undergoes a subsequent condensation reaction yielding the  $\text{C}_2\text{S}_4$  moiety. In this area of activation further work is underway in our group. One notable success in this regard, concerns the reaction of 6 with acetylenes

yielding complexes of the type  $[\text{Rh}_2\text{Cl}_2(\mu\text{-CO})(\mu\text{-acetylene})\text{-}(\text{DPM})_2]$  (8),<sup>42</sup> in which the acetylene molecule is activated, as seen by its structural parameters which resemble those of a cis dimetallated olefin molecule. Furthermore, as a result of the reaction of 6 with acetylenes a catalytic study using complex 6 was initiated<sup>169</sup> and preliminary results show that this complex catalyzes the cyclotrimerization of dimethylacetylenedicarboxylate, whereas with phenylacetylene, catalytic hydrogenation is observed.

## REFERENCES AND FOOTNOTES

1. M.M. Taqui Khan and A.E. Martell, "Homogeneous Catalysis by Metal Complexes", Academic Press, New York, 1974.
2. B.R. James, "Homogeneous Hydrogenation", Wiley, New York, 1973.
3. "Homogeneous Catalysis", Adv. Chem. Ser. No. 70, Chapters 1, 2, 4-7 and 10. A.C.S., Washington, D.C., 1968; D. Forster and J.F. Roth, eds., "Homogeneous Catalysis. II", Adv. Chem. Ser. No 132, A.C.S., Washington, D.C., 1974.
4. G.N. Schrauzer, "Transition Metals in Homogeneous Catalysis", Marcel Dekker, Inc., New York, 1971.
5. P.M. Henry, Adv. Organometal. Chem. (1975), 13, 363.
6. P.M. Henry, J. Am. Chem. Soc. (1972), 94, 4437 and references therein.
7. G. Yagupsky, C.K. Brown and G. Wilkinson, J. Chem. Soc. A. (1970), 1392; (1970), 2753, and references therein.
8. J.F. Roth, J.H. Craddock, A. Hershman and F.E. Paulick, Chem. Tech. (1971), 600.
9. D. Forster, J. Am. Chem. Soc. (1976), 98, 846.
10. R. Eisenberg and D.E. Hendricksen, Adv. Catal. (1979), 28, 79, and references therein.
11. E.L. Muetterties, Bull. Soc. Chim. Belg. (1975), 84, 959.



12. S.D. Ittel and J.A. Ibers, Adv. Organometal. Chem. (1976), 14, 33.
13. M.J.S. Dewar, Bull. Soc. Chim. (1951), 18, 79.
14. J. Chatt and L.A. Duncanson, J. Chem. Soc. (1953), 2939.
15. J.A.J. Jarvis, B.T. Kilbourn and P.G. Owston, Acta Crystallogr., Sect. B (1971), 27, 366.
16. F.R. Hartley, Agnew. Chem. Internat. Edit. (1972), 11, 596, and references therein.
17. W.P. Hayes and A.J. Forney, "High BTU Gas from Coal: Status and Prospects", Tech. Rep. PERC/IC-76-1 U.S.E.R.D.A., Office of Public Affairs, 1976.
18. R.E. Kirk and Othmer, eds., "Encyclopedia of Chemical Technology", 2nd ed., Wiley (Interscience), New York, 1963-1970. For CO/H<sub>2</sub> reaction, see Vol. 4, p. 446 for methanation, see Vol. 13, p. 364.
19. H. Pichler and H. Schulz, Chem. Ing. Tech. (1970), 42, 1162.
20. H.H. Storch, H. Golumbic and R.B. Anderson, "The Fischer-Tropsch and Related Syntheses", Wiley, New York, 1951.
21. F. Fischer and H. Tropsch, Chem. Ber. (1923), 56, 2428; (1926), 59, 830, 832, 923.
22. D.A. Edge and J.S. Adams, J.S. Afr. Inst. Min. Metall. (1975), 76, 145.

23. F.C. Palilla, U.S. Patent 3931393.
24. J. Freiberg, Atmos. Environ. (1976), 10, 121.
25. D.G. Jones and K.S. Campbell, AICHE Symp. Ser. (1975) 71, 306.
26. P.T. Roberts and S. Friedlander, Environ. Health Perspect. (1975), 103.
27. A.J. Chalk and R.F. Harrod, Adv. Organometal. Chem. (1968), 6, 119.
28. I. Wender and P. Pino, eds., "Organic Synthesis via Metal Carbonyls," Vol. 1, Wiley (Interscience), 1968.
29. R. Colton and M.J. McCormick, Coord. Chem. Rev. (1980), 31, 1, and references therein.
30. a) L. Vaska, Science (1966), 152, 769.  
b) N. Payne and J.A. Ibers, Inorg. Chem. (1969), 8, 2714.
31. J.T. Mague, Inorg. Chem. (1969), 8, 1975.
32. R. Colton, M.J. McCormick and C.D. Pannan, J. Chem. Soc. Chem. Comm. (1977), 823; Aust. J. Chem. (1978), 31, 1425.
33. F.A. Cotton and J.M. Troup, J. Am. Chem. Soc. (1974), 16, 4422.
34. P. Singh, C.B. Damman and D.J. Hodgson, Inorg. Chem. (1972), 12, 1335.
35. a) M. Cowie, J.T. Mague and A.R. Sanger, J. Am. Chem. Soc. (1978), 100, 3628.  
b) M. Cowie, Inorg. Chem. (1979), 18, 286, and references therein.

36. Y. Degreve, J. Meunier-Piret, M. van Meerssche and P. Piret, Acta Crystallogr., Sect. B. (1969), 25, 519.
37. C.J. Commons and B.F. Hoskins, Aust. J. Chem. (1975), 28, 1663.
38. V.G. Albano, P.L. Bellon, P. Chini and V. Scatturin, J. Organometal. Chem. (1969), 16, 461.
39. F.A. Cotton and D.L. Hunter, Inorg. Chem. (1974) 13, 2044.
40. P.S. Batterman, Strut. Bonding (Berlin) (1972), 10, 1.
41. M.P. Brown, A.N. Keith, Lj. Manojlovic-Muir, K.W. Muir, R.J. Puddephatt and K.R. Seddon, Inorg. Chim. Acta (1979), 34, L223.
42. M. Cowie and T.G. Southern, J. Organometal. Chem., in press.
43. I.S. Butler and A.E. Fenster, J. Organometal. Chem. (1977), 66, 161.
44. P.V. Yaneff, Coord. Chem. Rev. (1977), 23, 183.
45. M.C. Baird, G. Hartwell, R. Mason, A.I.M. Rae and G. Wilkinson, Chem. Comm. (1967), 92.
46. J.M. Lisey, E.D. Dobrzynski, R.J. Angelici and J. Clardy, J. Am. Chem. Soc. (1975), 97, 656.
47. T.G. Southern, D.Sc. Thesis, L'Université de Renne, 1979.
48. M.C. Baird and G. Wilkinson, J. Chem. Soc. A (1967), 865.

49. M. Kubota and C.R. Carey, J. Organometal. Chem., (1970), 24, 491.
50. T. Herskovitz and J. Guggenberger, J. Am. Chem. Soc. (1976), 98, 1615.
51. M. Aresta and G.F. Nobile, J. Chem. Soc. Dalton (1977), 708.
52. D.M.P. Mingos, Transition Met. Chem. (1978) 3, 1.
53. G.J. Kubas, Inorg. Chem. (1979), 18, 182.
54. D.C. Moody and R.R. Ryan, Inorg. Chem. (1979), 18, 223.
55. R.R. Ryan, P.G. Eller and G.J. Kubas, Inorg. Chem. (1976), 15, 797.
56. S.J. LaPlaca and J.A. Ibers, Inorg. Chem. (1966), 5, 405.
57. G.J. Kubas and R.R. Ryan, Cryst. Strut. Comm. (1977), 6, 295.
58. D.C. Moody and R.R. Ryan, J. Chem. Soc., Chem. Comm. (1976), 503; Inorg. Chem. (1977), 16, 2473.
59. R.D. Wilson and J.A. Ibers, Inorg. Chem. (1978), 17, 2134.
60. M. Angoletta, P.L. Bellon, M. Manssero and M. Sansoni, J. Organometal. Chem. (1974), 81, C40.
61. M. Angoletta, L. Malatesta and G. Caglio, J. Chem. Soc., Dalton (1977), 2131.
62. J.W. Moore, H.W. Baird and H.B. Miller, J. Am. Chem. Soc. (1968), 90, 1358.

63. a) B.L. Haymore and J.A. Ibers, Inorg. Chem. (1975), 14, 2610.  
b) B.A. Frenz and J.A. Ibers, M.T.P. Int. Rev. Sci., Phys. Chem. Ser. One (1973), 11, 33.
64. M.R. Churchill, B.G. DeBoer and K.L. Karla, Inorg. Chem. (1973), 12, 1650.
65. M.R. Snow and J.A. Ibers, Inorg. Chem. (1973), 12, 224.
66. J.T. Mague and J.P. Mitchner, Inorg. Chem. (1969), 8, 119.
67. L. Vallarino, J. Chem. Soc. (1957), 2287.
68. L. Vaska and J.W. Diluzio, J. Am. Chem. Soc. (1961), 83, 2784.
69. L. Vaska, Acc. Chem. Res. (1968), 1, 335.
70. J.P. Collman and W.R. Roper, Adv. Organometal. Chem. (1968), 7, 53.
71. A.L. Balch and B. Tulyathan, Inorg. Chem. (1977), 16, 2840.
72. M. Brockhaus, F. Standacher and H. Vahrenkamp, Chem. Ber. (1972), 105, 3716; L.R. Nassimbeni, Inorg. Nucl. Chem. Lett. (1971), 7, 187.
73. E.W. Ainscough, A.M. Brodie and G. Leng-Ward, J. Chem. Soc., Dalton (1974), 2437.
74. H. Vahrenkamp, Chem. Ber. (1972), 105, 3574.
75. a) J.A. Connor and G.A. Hudson, J. Organometal. Chem. (1974), 73, 351.

- b) J.A. Connor, G.K. McEwan and C.J. Rix, J. Less Common Metals (1974), 36, 207; J. Chem. Soc., Dalton (1974), 589.
76. J.A. Connor, J.P. Day, E.M. Jones and G.K. McEwan, J. Chem. Soc., Dalton (1973), 347; S.C. Tripathi, S.C. Srivastava and A.K. Shrimal, J. Organometal. Chem. (1976), 73, 343.
77. A.J. Pryde, B.L. Shaw and B. Weeks, J. Chem. Soc., Dalton (1976), 322.
78. J.P. Crow, W.R. Cullen, F.L. Hou, L.Y.Y. Chan and F.W.B. Einstein, J. Chem. Soc., Chem. Comm. (1971) 1229.
79. J.P. Crow, W.R. Cullen and F.L. Hou, Inorg. Chem. (1972), 11, 2125.
80. R. Colton and C.J. Commons, Aust. J. Chem. (1975), 28, 1673.
81. a) A.L. Balch and L.S. Benner, J. Organometal. Chem. (1977), 135, 339.  
b) L.S. Benner, M.M. Olmstead and A.L. Balch, J. Organometal. Chem. (1978), 159, 289.
82. A.R. Sanger, J. Chem. Soc., Dalton (1977), 1971.
83. a) M.P. Brown, R.J. Puddephatt, M. Rashidi and K.R. Seddon, J. Chem. Soc., Dalton (1977), 951.  
b) M.P. Brown, R.J. Puddephatt, M. Rashidi, Lj. Manojlović-Muir, K.W. Muir, T. Solomun and K.R. Sheddon, Inorg. Chim. Acta (1977), 23, L33.

84. A.L. Balch and L.S. Benner, J. Am. Chem. Soc. (1978) 100, 6099.
85. a) L.S. Benner, M.M. Olmstead, H. Hope and A.L. Balch, J. Organometal. Chem. (1978), 153, C31.  
b) A.L. Balch, L.S. Benner and M.M. Olmstead, Inorg. Chem. (1979), 18, 2996.
86. A.D. Rattray and D. Sutton, Inorg. Chim. Acta (1978), 27, L85.
87. A.L. Balch, C.L. Lee, C.H. Lindsay and M.M. Olmstead, J. Organometal. Chem. (1979), 177, C22.
88. a) M.P. Brown, J.R. Fisher, S.J. Franklin and R.J. Puddephatt, J. Chem. Soc., Chem. Comm. (1978), 749.  
b) M.P. Brown, J.R. Fisher, R.J. Puddephatt and K.R. Seddon, Inorg. Chem. (1979), 18, 2808.
89. C.P. Kubiak and R. Eisenberg, J. Am. Chem. Soc. (1978), 100, 3628.
90. M.M. Olmstead, L.S. Benner, H. Hope and A.L. Balch, Inorg. Chim. Acta (1979), 32, 193.
91. J.T. Mague and A.R. Sanger, Inorg. Chem. (1979), 18, 2060.
92. G.H. Stout and L.H. Jensen, "X-ray Structure Determination", 3rd ed., The MacMillan Company, Toronto, Canada, 1970.
93. M.J. Burger, "Crystal Structure Analysis", Wiley, New York, 1960.
94. M.J. Burger, "Vector Space", Wiley, New York, 1959.

95. "International Tables for X-ray Crystallography", 3rd Ed., The Kynoch Press, Birmingham, England, Vol. I, II, III and IV, 1974.
96. a) M. Cowie, S.K. Dwight and A.R. Sanger, Inorg. Chim. Acta (1978), 31, L407.  
b) M. Cowie and S.K. Dwight, Inorg. Chem. (1980), 19, 209.
97. M. Cowie and S.K. Dwight, unpublished results.
98. A.R. Sanger, private communication.
99. J. Chatt and L.M. Venazzi, J. Chem. Soc. (1957), 4735.
100. Positive  $^{19}\text{F}$  NMR shifts are upfield from  $\text{CFCl}_3$ .
101. Positive  $^{31}\text{P}$  NMR shifts are downfield from  $\text{H}_3\text{PO}_4$ .
102. The cell reduction was performed using a modification of TRACER II by S.L. Lawson. See: S.L. Lawson, R.A. Jacobson, "The Reduced Cell and Its Crystallographic Applications", Ames Laboratory Report IS-1141; USEAC: Iowa State University, Ames, Iowa, April, 1965.
103. R.J. Doedens and J.A. Ibers, Inorg. Chem. (1967) 6, 204.
104. A.L. Patterson, Phys. Rev. (1934), 46, 372.
105. A.L. Patterson, Z. Kristallogr., Sect. A. (1935), 90, 517.
106. D.T. Cromer, J.T. Waber, "International Tables for X-ray Crystallography", The Kynoch Press, Birmingham, England (1974), Vol. IV, Table 2.2A.




107. R.F. Stewart, E.R. Davidson and W.T. Simpson, J. Chem. Phys. (1965), 42, 3175.
108. D.T. Cromer and D.J. Liberman, J. Chem. Phys. (1970), 53, 1891.
109.  $f_o^{\text{anom}} = f_o + \Delta f' + i\Delta f''$ , where  $f_o$  is the normal scattering factor,  $\Delta f'$  is the real correction term and  $\Delta f''$  is the imaginary component.
110. Supplementary material is available from the National Library of Canada, 395 Wellington St., Ottawa, Ontario, K1A 0N4.
111. B.L. Haymore and J.A. Ibers, Inorg. Chem. (1975), 14, 1369; S.D. Ittel and J.A. Ibers, ibid. (1975), 14, 636; P.H. Davis, L.K. White and R.L. Belford, ibid. (1975), 14, 1753; R.E. Crommer, W. Van Doorne and R. Dubois, ibid. (1975), 14, 2462; D.S. Milbraith, J.P. Springer, J.C. Cardy and J.G. Verkade, ibid. (1975), 14, 2665.
112. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 3rd Ed., Wiley (Interscience), New York, (1972), pg. 120.
113. L.F. Dahl, C. Martell and D.L. Wampler, J. Am. Chem. Soc. (1961), 83, 1761.
114. J.A. Ibers and R.G. Snyder, Acta Crystallogr., Sect. B. (1962), 15, 923.
115. J.J. Bonnet, Y. Jeanin, P. Kalck, A. Maisonnet and R. Poilblanc, Inorg. Chem. (1975), 14, 743.

116. J. Coetzer and G. Gafner, Acta Crystallogr., Sect. B (1970), 26, 985.
117. M.J. Bennett and P. Donaldson, Inorg. Chem. (1977), 16, 655.
118. G. Holloway, B.R. Penfold, R. Colton and M.J. McCormick, J. Chem. Soc., Chem. Comm. (1976), 485.
119. J.T. Mague and A.R. Sanger, private communication.
120. M. Cowie and S.K. Dwight, Inorg. Chem. (1979), 18, 2700.
121.  $R = \Sigma ||F_O| - |F_C|| / \Sigma |F_O|$  ;  
 $R_w = [\Sigma (|F_O| - |F_C|)^2 / \Sigma F_O^2]^{1/2}$
122. J.L. DeBoer, D. Rogers, A.C. Shapski and P.G.H. Troughton, Chem. Comm. (1966), 756.
123. M.J. Bennett, P.B. Donaldson, P.B. Hitchcock and R. Mason, Inorg. Chim. Acta. (1975), 12, L9.
124. For average quantities the estimated standard deviation shown is the larger of an individual standard deviation or the standard deviation of a single observation from the mean.
125. M. Cowie and S.K. Dwight, to be submitted for publication.
126. M. Cowie and S.K. Dwight, Inorg. Chem. (1980), in press.
127. P. Singh, C.B. Dammann and D.J. Hodgson, Inorg. Chem. (1973), 12, 1335.
128. J. Donohue, "The Structures of the Elements", Wiley, New York, (1974), p. 216.

129. E.R. Corey, L.F. Dahl and W.J. Beck, J. Am. Chem. Soc. (1963), 85, 1202.
130. O.S. Mills and J.P. Nice, J. Organometal. Chem. (1967), 10, 337.
131. O.S. Mills and E.F. Paulus, J. Organometal. Chem. (1967), 10, 331.
132. E.F. Paulus, Acta Crystallogr., Sect. B (1969), 25, 2206.
133. C.H. Wei, Inorg. Chem. (1969), 8, 2384.
134. M. Meunier-Piret, P. Piret and M. Van Meerssche, Bull. Soc. Chim. Belg. (1967), 76, 374.
135. M.R. Churchill and K.L. Karla, Inorg. Chem. (1973), 12, 1650.
136. R.R. Ryan and D.C. Moody, Inorg. Chem. (1977), 16, 1052.
137. M.R. Churchill, B.G. DeBoer, K.L. Karla, P. Reich-Rohrwig and A. Wojcicki, J. Chem. Soc., Chem. Comm. (1972), 981.
138. S. Otsuka, Y. Tatsuno, M. Miki, T. Aoki, M. Matsumoto, H. Yoshioka and K. Nakatsu, J. Chem. Soc., Chem. Comm. (1973), 445.
139. B. Post, R.S. Schewartz and I. Rankuchen, Acta Crystallogr. (1952), 5, 372.
140. K.W. Muir and J.A. Ibers, Inorg. Chem. (1969), 8, 1921.

141. M. Cowie and S.K. Dwight, Inorg. Chem. (1979), 18, 1209.
142. M.M. Olmstead, C.H. Lindsay, L.S. Benner and A.L. Balch, J. Organometal. Chem. (1979), 179, 289.
143. A.L. Balch, private communication.
144. M. Cowie and S.K. Dwight, Inorg. Chem. (1980), in press.
145. R.J. Haines, private communication.
146. A.R. Sanger, J. Chem. Soc., Chem. Comm. (1975), 893.
147. A.R. Sanger, J. Chem. Soc., Dalton (1977), 122.
148. G. Germain, P. Main and M.M. Woolfson, Acta Cryst-allogr., Sect. A. (1971), 27, 368.
149. M.R. Churchill and S.A. Julis, Inorg. Chem. (1978), 17, 3011.
150. C. Nave and M.J. Trutter, J. Chem. Soc., Dalton (1973), 2202.
151. M. Benard, Inorg. Chem. (1979), 18, 2782.
152. A. Mitschler, B. Rees and M.S. Lehman, J. Am. Chem. Soc. (1978), 100, 3390.
153. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 3rd Ed., Wiley (Interscience), New York, (1972), pg. 707.
154. M. Cowie, R.S. Dickson and T.G. Southern, unpublished results.
155. All carbonyl vibrations are quoted for natural abundance CO.

156. R. Mason and A.I.M. Rae, J. Chem. Soc. A (1970), 1767.
157. T. Kushiwagi, N. Yasuoka, T. Ueki, N. Kasai, M. Kakuda, S. Takahashi and N. Hagihara, Bull. Chem. Soc. Jap. (1968), 41, 296.
158. H. Werner, K. Leonhard and Ch. Burschka, J. Organometal Chem. (1978), 160, 291.
159. H. LeBozec, P.H. Dixneuf, A.J. Carty and N.J. Taylor, Inorg. Chem. (1978), 17, 2568.
160. M. Aresta, C.F. Nobile, V.G. Albano, E. Forni and M. Manassero, J. Chem. Soc., Chem. Comm. (1975), 636.
161. D. Commereuc, I. Douek and G. Wilkinson, J. Chem. Soc. A (1970), 1771.
162. a) H. Werner, O. Kolb, R. Feser and U. Schubert, J. Organometal. Chem. (1980), 191, 283.  
b) H. Werner, private communication
163. M. Cowie and J.A. Ibers, Inorg. Chem. (1976), 15, 552.
164. K. Itoh, I. Matsuda, F. Ueda, Y. Ishii and J.A. Ibers, J. Am. Chem. Soc. (1978), 99, 2118.
165. B. Cetinkaya, M.F. Lappert, G.M. McLaughlin and K. Turner, J. Chem. Soc., Dalton (1974), 1591.
166. "International Tables for X-ray Crystallography", 3rd Ed., The Kynoch Press, Birmingham, England, Vol. III, (1972), pg. 276.
167. R. Beckett, and B.F. Hopskin, Inorg. Nuc. Chem. Lett. (1972), 8, 683.

168. V.R. Richter, J. Kaiser, J. Sieler and L. Kutschabsky,  
Acta Crystallogr., Sect. B (1975), 31, 1642.
169. M. Cowie and T.G. Southern, unpublished results.
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Appendix 1: Programs Used in Crystal Structure Solution,  
Refinement and Analysis.

<u>Author</u>	<u>Program</u>	<u>Description</u>
Northwestern University Version	AGNOST	Absorption correction program using Gaussian integration.
J.A. Ibers A.P. Gaughan	CELREF	Refines crystal alignment and cell parameters.
S.K. Dwight	DATABL	Outputs tables of posi- tion and thermal para- meters for publication.
A. Zalkin	FORDAP	Fourier summation for Patterson or Fourier maps.
P.D. Cradwick	HATOM	Calculates positions of hydrogen atoms attached to atoms which are $sp^3$ or $sp^2$ hybridized.
M.J. Bennett B. Foxman	MMMR	Calculates starting para- meters for rigid bodies and hindered rotors.
G. Germain P. Main M.M. Woolfson	MULTAN	General direct methods program.
P. Main C.T. Grainger	NORMAL	Calculates E's, does Wilson statistics. For input to MULTAN.
M.E. Pippy F.R. Ahmed	NRC-22	Calculates least-squares planes.

## Appendix 1, continued

<u>Author</u>	<u>Program</u>	<u>Description</u>
W. Busing H.A. Levy	ORFFE	Calculates bond lengths, angles and associated standard deviations. Modified by W.L. Brooks and M. Elder for hindered rotors and rigid bodies.
C. Johnson	ORTEP	Thermal ellipsoids plotting program.
M.J. Bennett	PMMO	Transforms raw data to intensities, applying corrections.
A.P. Gaughan	PRCNTA	Molecular weight, % composition, density, absorption coefficient calculations from formula and cell.
M. Cowie	PUBE	Sorts data according to any desired sequence of h, k or l.
R.C. Elder	PUBTAB	Prints structure factor amplitude tables, modified by S.K. Dwight for use on the page printer.
S.K. Dwight	RIGIDH	Calculated rigid body parameters for hydrogen atoms.



## Appendix 1, continued

<u>Author</u>	<u>Program</u>	<u>Description</u>
C.T. Prewitt	SFLS5	Structure factor calculation and least-squares refinement of parameters. Modified by B.M. Foxman and M.J. Bennett for rigid body routine, and by W.L. Hutcheon and M.J. Bennett for the hindered rotor.
S.L. Lawton	TRACERA	General Cell Reduction Program.

Appendix 2: Structure Factor Amplitudes for  
[Rh<sub>2</sub>(CO)<sub>2</sub>(μ-Cl)(DPM)<sub>2</sub>][BF<sub>4</sub>], *trans*-[RhCl(CO)-  
(DPM)]<sub>2</sub>, [Rh<sub>2</sub>Cl<sub>2</sub>(μ-SO<sub>2</sub>)(DPM)<sub>2</sub>], [Rh<sub>2</sub>Br<sub>2</sub>(μ-CO)-  
(DPM)<sub>2</sub>] and [Rh<sub>2</sub>Cl<sub>2</sub>(CO)(C<sub>2</sub>S<sub>4</sub>)(DPM)<sub>2</sub>].

Table 41. 10\*(Fobs vs. Fcal) For [Rh2(CO)2(mu-C1)(DPM)2][BF4].

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -14****															
1	-3	91	78	1	-5	184	202	7	1	250	242	4	3	306	289
1	0	107	107	1	-4	588	591	7	2	101	133	4	5	116	121
1	1	207	185	1	-3	632	636	7	3	330	331	4	6	209	210
1	2	403	408	1	-2	323	316	7	4	160	166	4	7	428	424
1	3	375	352	1	0	215	233	8	-3	217	215	4	8	399	402
1	4	135	147	1	1	601	598	8	-2	109	112	5	-6	126	122
2	-2	86	76	1	2	638	640	8	1	359	347	5	-5	138	116
2	0	168	171	1	3	228	237	8	2	463	452	5	-4	131	136
2	1	447	451	1	5	270	260	**H = -11****				5	-2	118	93
2	2	399	390	1	6	224	261	1	-8	322	327	5	-1	88	82
2	3	143	150	1	7	133	135	1	-7	211	196	5	0	120	127
3	-2	133	133	2	-5	321	318	1	-6	103	118	5	1	253	262
3	-1	78	60	2	-4	371	360	1	-5	235	234	5	3	330	296
3	0	101	109	2	-2	130	143	1	-3	620	630	5	4	309	303
3	2	247	234	2	-1	140	160	1	-2	612	606	5	5	228	247
**H = -13****				2	0	345	333	1	-1	368	381	5	6	158	163
1	-6	138	148	2	1	315	293	1	2	372	369	5	8	217	192
1	-4	128	131	2	3	309	317	1	3	468	485	6	-5	107	103
1	-3	98	76	2	4	342	340	1	4	211	215	6	-3	261	251
1	0	236	234	2	5	159	174	1	5	155	141	6	-2	441	449
1	1	392	387	3	-7	80	68	1	6	106	130	6	-1	184	169
1	2	108	89	3	-6	201	199	1	8	266	255	6	0	108	104
1	3	306	295	3	-4	327	349	1	9	331	347	6	1	304	306
1	4	357	348	3	-3	574	593	2	-8	329	338	6	2	660	670
1	5	234	230	3	-2	379	383	2	-7	152	136	6	3	634	593
1	6	199	188	3	-1	100	87	2	-5	133	106	6	4	241	230
2	-4	330	334	3	0	93	105	2	-4	676	677	6	5	93	55
2	-3	382	371	3	1	111	96	2	-3	741	746	6	6	177	178
2	-2	221	225	3	2	219	227	2	-2	248	253	6	7	277	297
2	-1	146	161	3	3	134	126	2	-1	142	148	7	-5	206	230
2	0	110	85	3	4	129	138	2	0	225	217	7	-4	380	348
2	1	265	295	3	6	79	73	2	1	301	299	7	-3	343	372
2	2	552	545	3	7	158	175	2	2	205	231	7	0	268	292
2	3	448	457	4	-6	261	258	2	5	118	106	7	1	485	531
2	4	184	181	4	-5	419	418	2	6	97	96	7	2	468	465
2	6	117	111	4	-4	106	112	2	7	116	122	7	3	149	141
3	-5	296	303	4	-3	172	194	2	8	131	108	7	4	173	164
3	-4	309	312	4	3	90	88	3	-8	170	149	7	5	237	249
3	-3	213	221	4	4	96	114	3	-7	119	107	7	6	238	250
3	0	249	254	4	6	129	117	3	-6	211	208	8	-6	96	123
3	1	385	367	5	-6	173	193	3	-5	348	345	8	-5	342	322
3	2	280	286	5	-5	93	83	3	-4	98	83	8	-4	285	293
3	5	86	85	5	-3	92	80	3	-1	283	277	8	-3	96	91
4	-3	307	300	5	-2	108	86	3	0	119	118	8	-2	248	256
4	-2	375	345	5	1	122	105	3	1	122	138	8	-1	223	196
4	-1	131	109	5	2	369	385	3	2	102	84	8	0	291	300
4	0	85	66	5	3	342	353	3	3	307	283	8	1	197	192
4	3	129	124	5	6	174	157	3	4	93	43	8	2	133	106
5	-4	354	323	6	-5	81	65	3	7	155	129	8	3	287	271
5	-3	198	208	6	-3	101	90	3	8	521	515	8	4	266	275
5	-2	201	202	6	1	416	398	3	9	512	544	8	5	163	177
5	0	137	103	6	2	483	483	4	-8	215	225	9	-4	329	344
6	-2	81	90	6	3	216	212	4	-7	88	86	9	-3	337	335
6	1	124	122	6	5	196	201	4	-6	226	203	9	-2	106	78
6	2	101	84	7	-4	81	65	4	-2	83	52	9	-1	86	90
**H = -12****				7	-2	110	106	4	1	275	299	9	1	176	192
				7	0	199	200	4	2	511	523	9	2	217	205

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -11****				4	-1	94	89	9	-1	141	156	3	-6	136	143
9	3	130	142	4	2	383	406	9	0	50	157	3	-5	114	111
9	4	110	91	4	3	632	638	9	1	16	90	3	-3	485	456
10	0	119	121	4	4	471	469	9	3	185	176	3	-2	477	508
**H = -10****				4	5	149	156	9	5	168	179	3	0	311	288
1	-10	331	326	4	8	446	388	10	-5	90	76	3	1	456	463
1	-9	531	541	4	9	326	346	10	-4	140	155	3	2	884	880
1	-8	317	300	5	-5	172	156	10	-3	117	94	3	3	875	854
1	-6	219	241	5	-4	453	479	10	0	82	93	3	4	458	473
1	-5	368	360	5	-3	587	579	10	1	243	233	3	6	236	219
1	-4	634	631	5	-2	243	259	10	2	303	263	3	7	343	339
1	-3	213	226	5	-1	176	184	10	3	100	110	3	8	450	439
1	-2	264	276	5	0	313	310	11	0	151	154	3	9	298	307
1	-1	405	392	5	1	616	629	11	1	258	262	4	-10	99	130
1	0	473	467	5	2	875	902	**H = -9****				4	-7	117	124
1	1	267	276	5	3	332	340	1	-10	95	118	4	-5	157	156
1	5	157	156	5	5	268	233	1	-9	549	546	4	-4	352	341
1	6	124	138	5	6	260	269	1	-8	738	711	4	-3	627	622
1	8	268	253	5	7	264	241	1	-7	527	507	4	-1	273	283
1	9	518	504	5	8	146	181	1	-5	293	290	4	0	228	242
1	10	459	466	6	-8	98	82	1	-4	428	429	4	1	498	530
2	-10	209	203	6	-6	184	167	1	-3	541	541	4	2	604	590
2	-9	159	147	6	-5	508	496	1	-2	298	310	4	3	89	49
2	-8	448	435	6	-4	381	380	1	-1	121	110	4	4	126	116
2	-7	414	420	6	-2	242	256	1	0	145	146	4	5	217	228
2	-6	221	246	6	-1	201	168	1	1	218	197	4	6	169	161
2	-3	352	380	6	0	385	406	1	2	540	540	4	7	132	80
2	-2	406	407	6	1	476	439	1	3	505	500	4	8	229	217
2	-1	328	323	6	3	222	216	1	4	103	73	4	9	88	100
2	2	199	207	6	4	304	290	1	5	113	76	5	-8	268	234
2	3	333	361	6	5	279	242	1	6	167	116	5	-7	135	138
2	4	182	192	6	6	185	163	1	7	547	545	5	-6	100	83
2	5	175	166	7	-8	128	115	1	8	654	677	5	-5	124	111
2	7	210	239	7	-6	168	196	1	9	216	186	5	-4	148	142
2	8	641	615	7	-3	548	580	1	10	311	300	5	-3	937	946
2	9	583	577	7	-2	518	525	1	11	331	335	5	-2	622	613
2	10	96	121	7	-1	187	195	2	-10	358	341	5	-1	178	192
3	-9	463	466	7	1	363	366	2	-9	408	396	5	1	146	120
3	-8	363	333	7	2	430	438	2	-8	167	175	5	2	589	578
3	-7	157	141	7	3	307	342	2	-6	322	324	5	3	567	565
3	-5	107	97	7	4	152	159	2	-5	454	426	5	4	241	234
3	-4	156	170	7	6	89	101	2	-4	127	95	5	6	181	145
3	-2	184	189	8	-6	99	115	2	-3	136	127	5	9	242	241
3	1	200	171	8	-5	364	375	2	-2	171	169	6	-9	426	421
3	2	426	437	8	-4	676	668	2	1	232	260	6	-8	366	354
3	3	95	81	8	-3	466	464	2	2	195	211	6	-7	164	162
3	4	299	284	8	0	346	347	2	3	413	438	6	-6	85	39
3	5	407	386	8	1	408	388	2	4	613	629	6	-5	218	212
3	6	364	347	8	2	174	192	2	5	341	360	6	-4	793	811
3	7	196	212	8	3	86	71	2	6	498	527	6	-3	797	825
3	8	125	115	8	4	98	89	2	8	445	440	6	-2	565	554
3	9	215	195	8	5	106	111	2	9	481	500	6	-1	116	90
3	10	214	222	8	7	226	208	2	10	393	390	6	0	269	279
4	-9	120	128	9	-6	117	102	2	11	168	176	6	1	534	514
4	-5	103	99	9	-5	198	200	3	-10	102	79	6	2	556	546
4	-3	160	180	9	-4	233	220	3	-8	143	119	6	3	276	257
4	-2	371	379	9	-3	101	106	3	-7	101	72	6	4	91	5

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-9****		12	0	241	269	4	-5	309	318	7	5	113	121
6	7	181	201	12	1	170	170	4	-4	469	465	7	6	241	207
6	8	273	259	12	2	128	113	4	-3	1191	1268	7	7	453	431
7	-9	377	377		**H =	-8****		4	-2	867	884	7	8	448	452
7	-6	258	240	1	-11	253	266	4	-1	119	133	7	9	124	101
7	-5	528	509	1	-10	294	286	4	1	348	374	8	-9	303	309
7	-4	383	388	1	-8	323	320	4	2	390	424	8	-7	242	239
7	-3	228	225	1	-7	412	438	4	3	491	474	8	-6	213	217
7	-2	213	217	1	-6	501	510	4	4	349	338	8	-5	252	262
7	-1	298	293	1	-5	146	146	4	5	245	229	8	-4	195	194
7	0	256	283	1	-4	293	300	4	6	103	82	8	-1	98	65
7	7	85	93	1	-3	110	106	4	9	183	185	8	0	114	91
7	8	280	277	1	-2	192	180	4	10	85	75	8	2	141	148
8	-8	327	349	1	-1	448	448	4	11	110	113	8	3	406	394
8	-7	267	265	1	0	176	156	5	-10	269	286	8	4	337	360
8	-6	151	169	1	1	501	462	5	-9	559	574	8	5	170	187
8	-4	225	228	1	2	268	280	5	-8	214	217	8	6	125	122
8	-3	435	447	1	3	1346	1365	5	-6	357	360	8	8	441	428
8	-2	362	362	1	4	1331	1318	5	-5	119	127	8	9	511	491
8	-1	208	199	1	5	535	530	5	-4	655	653	9	-9	168	158
8	1	120	104	1	7	246	254	5	-3	570	557	9	-8	165	190
8	2	187	170	1	8	993	951	5	-2	129	130	9	-7	203	190
8	3	297	311	1	9	759	763	5	-1	373	347	9	-6	136	121
8	4	140	132	1	10	310	310	5	0	186	193	9	-5	98	47
8	7	308	319	1	12	120	121	5	3	102	78	9	-4	99	124
8	8	612	599	2	-10	141	124	5	6	181	173	9	-2	278	276
9	-8	255	267	2	-9	393	365	5	8	160	173	9	-1	126	120
9	-7	77	80	2	-8	321	340	5	9	501	511	9	1	370	362
9	-6	109	93	2	-7	171	196	5	10	324	306	9	2	686	630
9	-5	108	165	2	-3	651	668	6	-10	278	290	9	3	653	671
9	-4	214	218	2	-2	445	474	6	-8	500	492	9	4	266	258
9	-3	173	184	2	1	438	443	6	-7	573	595	9	6	143	154
9	-2	160	141	2	2	762	785	6	-6	155	146	9	7	369	392
9	1	88	50	2	3	832	872	6	-5	342	342	9	8	406	397
9	2	113	104	2	5	348	333	6	-3	926	932	10	-4	350	334
9	3	88	101	2	6	98	86	6	-2	655	645	10	-3	169	151
9	4	159	149	2	7	419	408	6	-1	353	390	10	-2	248	241
9	6	112	156	2	8	338	352	6	0	153	122	10	-1	180	134
9	7	276	287	3	-10	111	97	6	3	212	201	10	0	136	156
10	-6	98	90	3	-6	126	75	6	4	228	242	10	1	333	332
10	-3	204	214	3	-5	166	159	6	6	111	121	10	2	271	258
10	1	157	162	3	-4	145	85	6	7	130	121	10	4	279	240
10	2	302	321	3	-3	156	145	6	8	687	696	10	5	146	152
10	3	526	513	3	-2	768	796	6	9	647	645	10	6	118	136
10	4	235	211	3	-1	491	505	6	10	176	177	10	7	121	121
11	-5	121	108	3	0	239	222	7	-10	282	291	11	-4	120	89
11	-4	354	353	3	1	391	386	7	-9	578	578	11	-3	489	469
11	-3	373	371	3	2	126	143	7	-8	528	533	11	-2	312	334
11	-1	115	111	3	3	559	572	7	-7	230	231	11	1	126	122
11	0	281	248	3	4	756	707	7	-5	96	101	11	2	368	374
11	1	473	484	3	5	276	288	7	-4	621	636	11	3	427	424
11	2	479	485	3	6	224	238	7	-3	317	302	11	4	117	104
11	3	178	178	3	8	230	194	7	-2	157	143	12	-5	355	354
11	4	104	114	4	-10	102	106	7	0	160	165	12	-4	616	605
12	-4	244	258	4	-9	288	300	7	2	430	426	12	-3	495	497
12	-2	228	246	4	-8	510	517	7	3	400	401	12	-1	160	142
12	-1	176	173	4	-7	266	254	7	4	86	22	12	0	232	255

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-8****		3	1	660	624	6	5	504	509	9	6	145	111
12	1	323	299	3	2	504	503	6	6	255	231	9	8	179	183
12	2	308	284	3	3	238	233	6	7	108	152	10	-9	195	200
12	3	87	75	3	5	222	188	6	8	275	249	10	-8	230	249
12	4	79	58	3	7	270	278	6	9	608	613	10	-6	102	87
13	-4	183	190	3	9	151	122	6	10	560	575	10	-5	264	235
13	-3	129	125	3	10	191	223	7	-11	172	196	10	-4	531	536
13	-2	225	229	3	11	221	196	7	-10	209	211	10	-3	401	428
13	-1	209	194	4	-12	99	106	7	-9	96	87	10	-2	498	505
13	0	131	111	4	-10	129	76	7	-8	407	409	10	-1	177	174
	**H =	-7****		4	-8	237	215	7	-7	595	595	10	0	141	157
1	-11	236	229	4	-7	532	507	7	-6	224	211	10	1	319	322
1	-10	364	360	4	-6	361	376	7	-5	145	134	10	2	514	537
1	-9	250	251	4	-5	135	130	7	-4	218	205	10	3	319	318
1	-5	244	228	4	-4	119	122	7	-3	139	122	10	4	118	90
1	-4	278	283	4	-3	213	210	7	-2	183	196	10	7	98	72
1	-3	470	480	4	-2	659	675	7	-1	116	113	11	-8	83	79
1	-2	357	312	4	-1	315	347	7	0	111	121	11	-7	138	103
1	-1	837	883	4	0	289	281	7	2	431	417	11	-6	214	208
1	0	605	647	4	1	254	256	7	3	1129	1110	11	-5	282	329
1	1	402	430	4	2	83	63	7	4	825	776	11	-4	484	486
1	2	329	331	4	3	147	114	7	5	279	233	11	-3	174	146
1	3	207	183	4	4	136	131	7	6	129	117	11	-2	172	164
1	4	883	928	4	6	98	87	7	7	311	321	11	-1	326	317
1	5	1227	1254	4	7	96	99	7	8	686	642	11	0	230	227
1	6	452	450	4	8	825	825	7	9	550	575	11	3	133	99
1	8	135	92	4	9	692	712	7	10	194	191	11	5	89	15
1	9	373	372	4	10	393	391	8	-10	234	243	11	7	79	74
1	10	267	268	4	11	68	70	8	-9	269	269	12	-7	180	196
1	12	73	44	5	-9	582	565	8	-8	247	260	12	-6	131	133
2	-12	169	163	5	-8	834	826	8	-7	178	183	12	-4	245	235
2	-11	151	168	5	-7	696	650	8	-6	96	59	12	-3	480	494
2	-10	191	177	5	-4	412	393	8	-4	159	187	12	-2	341	338
2	-8	157	143	5	-3	610	631	8	-3	183	187	12	-1	164	173
2	-7	378	382	5	-2	357	365	8	-2	181	199	12	0	92	76
2	-6	380	417	5	2	165	183	8	-1	347	350	12	1	143	121
2	-3	766	755	5	3	397	372	8	0	129	108	12	2	164	149
2	-2	1531	1574	5	5	116	156	8	1	285	291	12	4	160	136
2	-1	882	934	5	6	152	150	8	2	694	703	13	-5	267	268
2	0	281	311	5	7	324	269	8	3	461	489	13	-4	346	346
2	1	332	330	5	8	486	510	8	5	248	220	13	-3	153	148
2	2	582	590	5	9	291	235	8	6	296	299	13	-2	109	109
2	3	1188	1214	5	10	93	50	8	7	434	431	13	-1	78	63
2	4	911	941	5	11	223	205	8	8	158	147	13	0	102	113
2	5	324	298	6	-11	153	152	9	-10	124	115	13	1	76	93
2	8	115	78	6	-10	448	441	9	-8	96	83	13	2	207	203
2	12	67	57	6	-9	539	531	9	-6	158	187	13	3	81	72
3	-11	76	63	6	-8	250	207	9	-5	178	166	13	4	110	81
3	-9	293	270	6	-7	278	274	9	-4	99	74	14	-3	78	61
3	-8	409	402	6	-6	307	285	9	-3	384	391	14	-1	114	115
3	-7	371	385	6	-5	342	350	9	-2	477	491	14	1	123	139
3	-6	206	175	6	-4	230	236	9	-1	301	276		**H =	-6****	
3	-5	232	232	6	-2	134	105	9	0	137	121	1	-12	93	109
3	-4	524	543	6	1	102	126	9	2	193	213	1	-8	181	174
3	-3	1084	1107	6	2	306	320	9	3	517	520	1	-7	671	629
3	-2	639	651	6	3	112	101	9	4	365	361	1	-6	363	355
3	0	124	92	6	4	668	672	9	5	213	206	1	-5	432	408

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-6****													
1	-4	187	166	4	-11	136	107	6	6	287	327	10	-7	333	326
1	-3	1122	1132	4	-10	339	330	6	7	558	508	10	-6	108	80
1	-2	1717	1753	4	-9	533	557	6	8	315	303	10	-5	319	320
1	-1	740	756	4	-8	777	765	6	10	185	204	10	-4	133	138
1	0	87	47	4	-7	263	242	6	11	128	148	10	-3	370	384
1	1	343	390	4	-6	409	440	7	-11	268	267	10	-2	495	506
1	2	593	651	4	-5	266	245	7	-10	354	346	10	-1	358	360
1	3	1180	1185	4	-4	236	248	7	-9	178	178	10	0	164	178
1	4	544	526	4	-3	346	363	7	-7	121	90	10	1	95	118
1	5	193	165	4	-2	210	226	7	-6	123	127	10	4	190	186
1	6	245	270	4	-1	120	120	7	-5	144	125	10	7	92	103
1	7	228	221	4	1	118	152	7	-4	246	252	10	8	277	269
1	9	149	126	4	2	204	187	7	-3	249	246	11	-9	517	514
1	11	160	177	4	3	197	196	7	-2	165	188	11	-8	488	485
1	12	195	199	4	4	542	549	7	-1	403	377	11	-7	179	139
1	13	114	118	4	5	980	989	7	0	494	527	11	-6	114	114
2	-12	101	69	4	7	110	123	7	1	264	272	11	-5	182	162
2	-9	293	266	4	9	537	528	7	2	339	334	11	-4	428	422
2	-8	109	100	4	10	475	486	7	3	350	356	11	-3	386	375
2	-7	162	224	4	11	280	278	7	4	941	934	11	-2	156	175
2	-6	531	523	4	12	66	81	7	5	639	598	11	-1	143	145
2	-5	318	278	5	-12	282	295	7	6	301	361	11	2	242	229
2	-4	225	246	5	-11	216	237	7	8	266	283	11	3	179	183
2	-3	420	422	5	-10	260	259	7	9	282	253	11	5	116	120
2	-2	266	295	5	-9	124	154	7	10	187	189	11	6	241	258
2	-1	1138	1147	5	-8	208	205	8	-11	181	189	11	7	323	304
2	0	1000	998	5	-7	619	631	8	-8	125	136	12	-7	221	233
2	1	280	336	5	-6	218	240	8	-7	98	98	12	-6	239	255
2	2	192	180	5	-5	242	244	8	-5	177	186	12	-5	274	263
2	3	86	76	5	-3	137	130	8	-4	250	257	12	-4	94	125
2	4	265	272	5	-2	135	124	8	-3	1098	1119	12	-3	180	170
2	5	177	165	5	-1	148	135	8	-2	981	999	12	-1	89	94
2	9	335	344	5	0	79	78	8	-1	412	434	12	0	89	51
2	10	561	582	5	3	814	823	8	0	151	198	12	1	243	228
2	11	358	371	5	4	1241	1251	8	2	700	717	12	2	110	113
2	12	147	149	5	5	496	483	8	3	1075	1049	12	3	244	227
3	-12	135	134	5	6	116	101	8	4	698	692	12	4	350	332
3	-9	344	333	5	7	142	138	8	5	92	82	12	5	180	187
3	-8	666	682	5	8	893	871	8	7	195	176	13	-7	252	238
3	-7	1012	1020	5	9	745	767	8	8	279	282	13	-6	100	108
3	-6	455	456	5	10	391	379	9	-10	72	54	13	-4	129	135
3	-5	233	216	5	11	81	51	9	-9	243	225	13	-2	106	111
3	-4	149	137	6	-12	239	245	9	-8	167	136	13	-1	110	85
3	-3	549	572	6	-11	78	44	9	-5	131	88	13	2	386	392
3	-2	1060	1052	6	-10	169	151	9	-4	588	575	13	3	617	610
3	-1	548	563	6	-9	291	269	9	-3	466	484	13	4	276	284
3	0	105	92	6	-8	636	630	9	-2	101	80	13	5	74	18
3	1	209	210	6	-7	223	229	9	-1	146	150	14	-4	92	106
3	3	286	272	6	-5	119	128	9	1	293	290	14	-3	205	216
3	4	91	25	6	-3	348	351	9	2	567	571	14	-2	75	75
3	6	138	107	6	-2	706	736	9	3	199	153	14	1	255	230
3	7	133	94	6	-1	186	174	9	4	93	53	14	2	460	425
3	8	717	676	6	1	452	441	9	5	193	173	14	3	118	109
3	9	559	525	6	2	732	774	9	6	113	62			**H =	-5****
3	10	116	109	6	3	974	963	9	9	122	86	1	-12	150	146
3	12	137	124	6	4	328	350	10	-10	118	136	1	-10	204	187
				6	5	385	319	10	-8	198	206	1	-9	278	270

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-5****		3	-1	91	91	6	-8	129	121	9	-9	194	186
1	-8	138	123	3	1	294	291	6	-7	129	138	9	-8	565	536
1	-7	1063	1032	3	2	196	174	6	-5	280	324	9	-7	459	451
1	-6	1137	1176	3	3	586	566	6	-4	139	134	9	-6	110	135
1	-5	692	739	3	4	872	891	6	-3	233	251	9	-5	105	94
1	-4	324	335	3	5	842	872	6	-2	759	787	9	-4	102	39
1	-3	404	420	3	6	103	72	6	-1	1224	1267	9	-3	763	767
1	-2	1556	1591	3	8	209	223	6	0	579	563	9	-2	683	683
1	-1	1285	1356	3	9	667	650	6	1	165	142	9	-1	407	411
1	0	1348	1413	3	10	806	821	6	2	360	339	9	2	203	176
1	1	467	443	3	11	356	381	6	3	1060	1128	9	6	182	143
1	2	531	532	4	-13	467	468	6	4	1143	1112	9	7	170	165
1	3	357	367	4	-12	334	336	6	5	508	504	9	8	233	247
1	4	351	372	4	-11	105	114	6	6	176	217	9	9	350	345
1	5	442	419	4	-10	115	67	6	7	389	423	9	10	84	74
1	6	220	182	4	-9	124	147	6	8	267	244	10	-10	322	317
1	7	170	168	4	-8	599	551	6	9	165	135	10	-9	603	618
1	8	146	91	4	-7	333	304	7	-12	113	121	10	-8	356	368
1	9	552	570	4	-6	144	154	7	-10	135	116	10	-6	173	170
1	10	605	606	4	-5	268	278	7	-8	360	383	10	-5	291	302
1	11	156	157	4	-4	179	196	7	-7	332	315	10	-4	377	396
1	13	171	181	4	-3	158	166	7	-5	91	63	10	-3	364	350
2	-13	226	238	4	-2	595	592	7	-4	433	412	10	-2	96	99
2	-12	185	181	4	-1	143	144	7	-3	1056	1098	10	-1	249	256
2	-11	159	162	4	0	480	458	7	-2	1086	1132	10	1	96	107
2	-9	329	315	4	1	231	250	7	-1	268	256	10	3	95	45
2	-8	976	941	4	2	287	313	7	0	381	377	10	4	136	138
2	-7	927	946	4	3	968	970	7	1	625	606	10	5	155	145
2	-6	434	472	4	4	1133	1196	7	2	735	779	10	6	160	138
2	-5	336	332	4	5	222	274	7	3	648	672	10	7	103	116
2	-4	656	687	4	6	127	95	7	5	152	169	10	9	308	319
2	-3	1432	1447	4	7	168	167	7	6	262	223	11	-10	148	163
2	-2	902	945	4	8	496	503	7	7	258	227	11	-8	265	242
2	-1	223	240	4	9	624	619	7	8	167	142	11	-7	290	287
2	0	158	132	4	11	149	175	7	9	100	106	11	-6	165	138
2	1	416	416	4	12	66	78	7	10	95	88	11	-5	148	173
2	2	148	136	5	-11	194	197	7	11	152	126	11	-4	199	200
2	4	221	186	5	-10	301	277	8	-11	109	108	11	-1	149	139
2	6	190	195	5	-9	322	285	8	-9	348	360	11	1	155	115
2	7	270	311	5	-8	289	265	8	-8	122	103	11	2	295	323
2	8	376	363	5	-6	91	50	8	-7	269	269	11	3	665	690
2	9	198	178	5	-3	292	285	8	-6	261	261	11	4	478	468
2	10	486	488	5	-2	143	146	8	-5	190	181	11	5	178	143
2	11	565	585	5	-1	615	636	8	-4	417	425	11	7	275	257
2	12	374	408	5	0	701	712	8	-3	197	177	11	8	516	521
2	13	152	167	5	1	577	573	8	-2	352	378	12	-9	381	394
3	-12	194	179	5	2	726	714	8	-1	759	785	12	-8	324	310
3	-11	220	247	5	3	272	228	8	0	426	408	12	-5	117	143
3	-10	435	403	5	4	759	753	8	1	446	456	12	-3	167	166
3	-9	308	300	5	5	1150	1153	8	2	110	115	12	-2	168	174
3	-8	317	301	5	6	282	278	8	3	240	232	12	-1	133	156
3	-7	249	244	5	9	421	415	8	4	271	281	12	1	258	265
3	-6	338	297	5	10	447	445	8	5	172	210	12	2	563	556
3	-5	581	560	5	11	141	138	8	6	107	110	12	3	425	437
3	-4	174	191	6	-12	267	272	8	9	187	215	12	5	200	222
3	-3	185	214	6	-11	314	321	8	10	408	393	12	6	202	192
3	-2	221	188	6	-10	107	99	9	-11	114	134	12	7	325	325



Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -5****															
13	-8	84	77	2	-11	416	411	4	-1	1080	1124	7	-5	279	304
13	-7	83	90	2	-10	397	403	4	0	900	921	7	-3	635	675
13	-6	81	91	2	-9	169	175	4	1	124	140	7	-2	1197	1255
13	-4	108	136	2	-8	425	407	4	3	131	92	7	-1	1045	1099
13	-3	290	275	2	-7	1168	1181	4	4	1446	1419	7	0	219	227
13	-2	167	185	2	-6	1046	1036	4	5	967	1033	7	1	105	42
13	-1	385	369	2	-5	150	158	4	6	341	309	7	2	363	378
13	0	171	197	2	-4	169	170	4	7	147	154	7	3	631	619
13	1	166	159	2	-2	107	89	4	8	108	38	7	4	220	196
13	3	379	395	2	-1	161	161	4	9	366	378	7	5	98	91
13	4	470	471	2	0	131	150	4	10	334	312	7	6	165	175
13	5	278	289	2	1	237	261	4	11	177	166	7	7	411	366
13	6	102	102	2	2	138	131	4	13	116	86	7	8	323	273
14	-6	102	69	2	3	640	656	5	-13	305	291	7	9	630	614
14	-4	147	183	2	4	1533	1550	5	-12	263	247	7	10	383	403
14	-3	361	321	2	5	526	503	5	-10	146	137	7	11	96	77
14	-2	394	398	2	6	121	163	5	-8	217	220	8	-12	84	110
14	-1	125	138	2	7	276	270	5	-7	334	313	8	-10	98	101
14	2	446	445	2	8	477	465	5	-6	268	253	8	-9	383	362
14	3	509	512	2	9	784	784	5	-5	107	103	8	-8	894	891
14	4	170	177	2	10	581	589	5	-4	401	392	8	-7	624	633
15	-4	386	374	2	11	111	93	5	-3	975	1018	8	-4	665	645
15	-3	265	253	2	12	86	77	5	-2	1441	1477	8	-3	972	996
15	-1	82	70	2	13	114	128	5	-1	1085	1119	8	-2	965	988
15	0	132	144	3	-13	598	606	5	0	815	765	8	-1	141	158
15	1	217	220	3	-12	244	241	5	1	391	386	8	0	187	180
**H = -4****				3	-10	149	176	5	2	404	436	8	1	338	361
1	-13	329	345	3	-9	122	98	5	3	1045	1085	8	2	118	124
1	-12	82	73	3	-8	808	781	5	4	585	535	8	3	238	249
1	-11	92	75	3	-7	334	332	5	5	124	27	8	6	118	46
1	-10	231	195	3	-6	109	104	5	6	401	425	8	7	172	140
1	-9	441	477	3	-4	239	242	5	7	274	282	8	8	142	93
1	-8	1009	969	3	-3	301	315	5	10	96	79	8	10	270	289
1	-7	370	353	3	-2	169	181	5	12	164	154	8	11	344	360
1	-6	922	925	3	-1	241	228	6	-13	99	116	9	-10	250	217
1	-5	501	525	3	0	863	861	6	-9	186	193	9	-9	437	425
1	-4	490	459	3	1	440	450	6	-8	529	504	9	-7	370	376
1	-3	1090	1076	3	2	425	416	6	-7	161	176	9	-6	273	232
1	-2	76	85	3	3	943	942	6	-6	205	221	9	-5	153	101
1	-1	594	606	3	4	375	346	6	-5	537	504	9	-4	279	271
1	0	542	564	3	5	1234	1253	6	-4	741	736	9	-3	149	165
1	1	353	347	3	6	484	421	6	-3	754	780	9	-1	213	204
1	2	763	778	3	7	316	341	6	-2	207	211	9	0	212	238
1	3	153	116	3	8	208	196	6	-1	832	850	9	2	131	149
1	4	152	174	3	9	125	83	6	0	876	916	9	3	341	311
1	5	919	886	3	10	307	297	6	1	611	645	9	4	471	419
1	6	792	819	3	11	409	423	6	2	632	629	9	5	192	251
1	7	364	343	3	12	157	164	6	4	795	800	9	7	89	27
1	8	145	155	4	-11	291	297	6	5	388	386	9	8	255	262
1	9	349	341	4	-10	174	157	6	9	199	155	9	9	499	504
1	10	957	974	4	-9	337	357	6	10	224	248	9	10	573	579
1	11	973	980	4	-8	165	189	6	11	272	275	10	-9	285	276
1	12	425	430	4	-7	97	91	6	12	74	81	10	-8	509	528
1	13	76	99	4	-4	282	242	7	-9	154	148	10	-7	321	330
2	-13	300	304	4	-3	211	163	7	-8	332	299	10	-6	141	132
2	-12	396	415	4	-2	469	504	7	-7	829	846	10	-4	151	138
				4	-2	469	504	7	-6	469	457	10	-3	107	80

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-4****		14	-1	305	306	2	8	189	171	5	-4	328	341
10	-2	344	347	14	0	265	278	2	9	188	162	5	-3	882	852
10	-1	116	111	14	1	212	216	2	10	594	616	5	-2	784	832
10	2	551	562	14	3	161	164	2	11	451	471	5	-1	1422	1507
10	3	806	797	14	4	197	164	2	12	95	76	5	0	968	983
10	4	290	282	14	5	123	123	3	-13	281	280	5	2	165	165
10	5	265	228	15	-4	181	167	3	-12	277	284	5	3	664	681
10	6	241	245	15	-3	431	430	3	-11	222	205	5	4	656	646
10	7	221	231	15	-2	339	336	3	-10	266	223	5	5	289	258
10	8	355	345	15	-1	124	116	3	-8	144	187	5	7	123	145
10	9	281	278	15	1	124	102	3	-7	199	181	5	8	194	186
11	-10	226	222	15	2	222	232	3	-6	282	313	5	9	289	279
11	-9	318	298		**H =	-3****		3	-5	92	80	5	10	555	546
11	-8	136	145	1	-13	615	594	3	-4	365	389	5	11	173	193
11	-5	189	180	1	-12	826	872	3	-3	858	887	5	12	99	130
11	-4	303	305	1	-11	570	570	3	-2	1192	1228	6	-13	168	146
11	-3	188	191	1	-10	126	106	3	-1	1174	1230	6	-12	243	219
11	-2	366	380	1	-9	283	279	3	0	962	978	6	-9	206	188
11	1	282	282	1	-8	1043	1081	3	1	360	380	6	-8	1054	1028
11	2	411	381	1	-7	1346	1313	3	2	836	844	6	-7	1133	1106
11	3	153	117	1	-6	1029	990	3	3	720	677	6	-6	528	556
11	4	655	645	1	-5	125	111	3	4	1459	1499	6	-4	531	541
11	5	450	430	1	-4	528	546	3	5	648	646	6	-3	1011	1036
11	6	133	136	1	-3	798	856	3	6	97	106	6	-2	1530	1589
11	8	128	136	1	-2	700	732	3	7	217	164	6	-1	649	655
12	-8	152	151	1	-1	753	756	3	8	273	273	6	0	115	119
12	-6	100	73	1	0	260	282	3	9	408	405	6	1	302	306
12	-4	170	203	1	1	608	601	3	10	301	291	6	2	551	556
12	-3	383	374	1	2	576	586	3	11	170	187	6	3	264	248
12	-2	672	733	1	3	987	1002	3	12	109	112	6	5	119	121
12	-1	565	546	1	4	789	786	4	-13	340	346	6	6	170	177
12	0	183	183	1	5	183	156	4	-12	252	261	6	8	178	200
12	1	94	115	1	6	318	375	4	-11	93	37	6	9	559	527
12	2	564	570	1	7	873	857	4	-9	130	133	6	11	508	523
12	3	791	772	1	8	834	789	4	-8	245	217	6	12	314	344
12	4	598	580	1	9	530	545	4	-6	283	278	7	-13	248	253
12	5	101	92	1	11	579	590	4	-5	143	172	7	-12	101	91
12	6	137	130	1	12	465	484	4	-4	621	643	7	-11	83	65
12	7	239	230	1	13	170	178	4	-3	742	745	7	-10	231	208
13	-8	209	192	2	-13	506	518	4	-2	818	815	7	-9	617	588
13	-7	144	165	2	-11	431	358	4	-1	121	133	7	-8	715	669
13	-6	95	43	2	-9	363	400	4	0	757	802	7	-6	411	453
13	-5	141	129	2	-8	411	391	4	1	813	793	7	-5	700	706
13	-4	402	412	2	-7	305	335	4	2	340	274	7	-4	496	494
13	-3	522	535	2	-5	107	146	4	3	341	327	7	-3	265	256
13	-2	374	386	2	-4	325	333	4	4	138	127	7	-2	185	178
13	0	216	233	2	-3	186	218	4	5	243	202	7	-1	601	607
13	1	308	304	2	-2	206	214	4	6	565	592	7	0	308	333
13	2	500	509	2	-1	231	250	4	10	268	261	7	1	109	132
13	3	248	229	2	0	790	803	4	11	363	374	7	2	411	415
13	4	90	79	2	1	274	308	4	12	103	111	7	3	132	133
13	5	252	239	2	2	459	484	4	13	66	50	7	4	207	211
13	6	142	163	2	3	687	756	5	-9	172	184	7	5	547	506
14	-7	102	72	2	4	1124	1185	5	-8	149	117	7	6	516	518
14	-5	175	175	2	5	1261	1282	5	-7	602	639	7	9	626	603
14	-4	230	239	2	6	1026	1006	5	-6	704	738	7	10	854	875
14	-2	210	231	2	7	261	305	5	-5	843	852	7	11	450	436

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H =	-3****			10	10	145	147	**H =	-2****			K	L	FOBS	FCAL
7	12	123	133	11	-10	102	80	1	-14	226	234	3	-1	624	691
8	-12	269	261	11	-7	277	262	1	-12	456	472	3	0	1457	1519
8	-11	156	164	11	-5	127	127	1	-11	981	957	3	1	318	353
8	-10	92	128	11	-3	743	728	1	-10	233	213	3	2	81	44
8	-8	550	524	11	-2	1058	1069	1	-9	94	37	3	3	374	409
8	-7	977	981	11	-1	228	239	1	-8	108	135	3	4	233	205
8	-6	560	586	11	0	219	212	1	-7	530	552	3	5	927	954
8	-5	305	351	11	1	282	276	1	-6	387	444	3	6	704	697
8	-4	135	136	11	2	590	606	1	-4	902	939	3	7	348	319
8	-3	221	235	11	3	642	665	1	-3	723	759	3	8	244	240
8	-2	426	435	11	4	130	149	1	-2	82	38	3	9	158	135
8	-1	88	78	11	5	208	206	1	-1	1736	1819	3	10	258	250
8	1	100	98	11	6	234	248	1	0	1587	1691	3	11	369	337
8	2	171	163	11	8	139	140	1	1	1315	1286	4	-13	121	140
8	3	285	303	12	-9	208	195	1	2	66	15	4	-12	189	191
8	4	654	682	12	-8	156	183	1	3	175	162	4	-11	85	26
8	5	424	361	12	-6	168	177	1	4	2653	2753	4	-9	128	159
8	6	92	89	12	-5	295	310	1	5	1989	1982	4	-8	837	823
8	7	168	136	12	-4	475	440	1	6	843	860	4	-7	1358	1314
8	8	618	601	12	-3	238	225	1	7	88	86	4	-6	860	843
8	9	693	691	12	-2	329	331	1	8	605	590	4	-5	395	310
8	10	404	397	12	-1	663	673	1	9	541	538	4	-4	403	377
9	-12	200	196	12	0	254	281	1	10	550	552	4	-3	876	879
9	-10	139	114	12	1	177	161	1	11	161	157	4	-2	1290	1324
9	-9	316	300	12	2	156	154	1	12	96	129	4	-1	1220	1294
9	-8	569	562	12	3	319	303	2	-14	203	187	4	0	620	626
9	-7	376	354	12	4	397	394	2	-13	397	394	4	1	68	24
9	-6	110	139	12	5	196	208	2	-12	652	679	4	3	666	694
9	-5	96	90	12	7	91	125	2	-11	255	250	4	4	148	146
9	-4	204	207	13	-8	274	262	2	-10	349	328	4	5	530	489
9	-3	200	231	13	-7	305	293	2	-9	140	98	4	6	384	364
9	-2	224	207	13	-6	193	197	2	-8	215	197	4	7	298	320
9	-1	91	9	13	-5	186	178	2	-7	132	132	4	8	275	261
9	0	116	8	13	-3	498	522	2	-6	120	83	4	9	201	194
9	2	348	384	13	-2	604	628	2	-5	379	379	4	10	235	263
9	3	289	276	13	-1	408	412	2	-3	466	480	4	11	300	305
9	5	391	404	14	2	387	424	2	-2	1215	1303	4	12	334	354
9	6	360	346	14	3	303	278	2	-1	1541	1592	4	13	124	142
9	7	398	342	14	-8	430	439	2	0	206	140	5	-13	267	295
9	8	172	173	14	-7	177	158	2	1	2269	2383	5	-12	133	151
9	10	390	379	14	-5	213	216	2	2	171	184	5	-11	85	60
10	-11	121	124	14	-4	388	407	2	3	1401	1390	5	-10	166	164
10	-10	121	133	14	-3	535	523	2	4	830	851	5	-9	418	408
10	-9	158	133	14	-2	315	335	2	6	594	575	5	-8	865	856
10	-7	94	88	14	-1	188	206	2	7	479	472	5	-7	621	633
10	-3	119	141	14	1	296	288	2	8	238	221	5	-6	512	494
10	-2	547	608	14	2	186	191	2	12	152	145	5	-5	106	127
10	-1	610	607	14	4	76	60	3	-14	109	130	5	-4	441	458
10	2	132	111	15	-6	103	120	3	-13	273	271	5	-3	626	619
10	3	602	626	15	-5	136	130	3	-11	171	177	5	-2	361	360
10	4	838	834	15	-4	179	177	3	-7	109	111	5	-1	513	547
10	5	412	373	15	-2	252	257	3	-6	621	573	5	0	937	952
10	6	222	204	15	1	95	100	3	-5	264	273	5	1	330	335
10	7	127	116	15	3	135	142	3	-4	560	528	5	2	149	145
10	8	225	242	15	4	222	208	3	-3	454	486	5	4	380	327
10	9	354	331	16	0	77	91	3	-2	376	403	5	5	341	346
												5	6	477	450

FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**	10	10	145	147	**H =	-2****			K	L	FOBS	FCAL
133	11	-10	102	80	1	-14	226	234	3	-1	624	691
261	11	-7	277	262	1	-12	456	472	3	0	1457	1519
164	11	-5	127	127	1	-11	981	957	3	1	318	353
128	11	-3	743	728	1	-10	233	213	3	2	81	44
524	11	-2	1058	1069	1	-9	94	37	3	3	374	409
981	11	-1	228	239	1	-8	108	135	3	4	233	205
586	11	0	219	212	1	-7	530	552	3	5	927	954
351	11	1	282	276	1	-6	387	444	3	6	704	697
136	11	2	590	606	1	-4	902	939	3	7	348	319
235	11	3	642	665	1	-3	723	759	3	8	244	240
435	11	4	130	149	1	-2	82	38	3	9	158	135
78	11	5	208	206	1	-1	1736	1819	3	10	258	250
98	11	6	234	248	1	0	1587	1691	3	11	369	337
163	11	8	139	140	1	1	1315	1286	4	-13	121	140
303	12	-9	208	195	1	2	66	15	4	-12	189	191
682	12	-8	156	183	1	3	175	162	4	-11	85	26
361	12	-6	168	177	1	4	2653	2753	4	-9	128	159
89	12	-5	295	310	1	5	1989	1982	4	-8	837	823
136	12	-4	475	440	1	6	843	860	4	-7	1358	1314
601	12	-3	238	225	1	7	88	86	4	-6	860	843
691	12	-2	329	331	1	8	605	590	4	-5	395	310
397	12	-1	663	673	1	9	541	538	4	-4	403	377
196	12	0	254	281	1	10	550	552	4	-3	876	879
114	12	1	177	161	1	11	161	157	4	-2	1290	1324
300	12	2	156	154	1	12	96	129	4	-1	1220	1294
562	12	3	319	303	2	-14	203	187	4	0	620	626
354	12	4	397	394	2	-13	397	394	4	1	68	24
139	12	5	196	208	2	-12	652	679	4	3	666	694
90	12	7	91	125	2	-11	255	250	4	4	148	146
207	13	-8	274	262	2	-10	349	328	4	5	530	489
231	13	-7	305	293	2	-9	140	98	4	6	384	364
28	13	-6	193	197	2	-8	215	197	4	7	298	320
9	13	-5	186	178	2	-7	132	132	4	8	275	261
8	13	-3	498	522	2	-6	120	83	4	9	201	194
384	13	-2	604	628	2	-5	379	379	4	10	235	263
176	13	-1	408	412	2	-3	466	480	4	11	300	305
104	13	2	387	424	2	-2	1215	1303	4	12	334	354
146	13	3	303	278	2	-1	1541	1592	4	13	124	142
142	14	-8	430	439	2	0	206	140	5	-13	267	295
73	14	-7	177	158	2	1	2269	2383	5	-12	133	151
179	14	-5	213	216	2	2	171	184	5	-11	85	60
24	14	-4	388	407	2	3	1401	1390	5	-10	166	164
33	14	-3	535	523	2	4	830	851	5	-9	418	408
33	14	-2	315	335	2	6	594	575	5	-8	865	856
88	14	-1	188	206	2	7	479	472	5	-7	621	633
41	14	1	296	288	2	8	238	221	5	-6	512	494
08	14	2	186	191	2	12	152	145	5	-5	106	127
07	14	4	76	60	3	-14	109	130	5	-4	441	458
11	15	-6	103	120	3	-13	273	271	5	-3	626	619
26	15	-5	136	130	3	-11	171	177	5	-2	361	360
34	15	-4	179	177	3	-7	109	111	5	-1	513	547
73	15	-2	252	257	3	-6	621	573	5	0	937	952
04	15	1	95	100	3	-5	264	273	5	1	330	335
16	15	3	135	142	3	-4	560	528	5	2	149	145
42	15	4	222	208	3	-3	454	486	5	4	380	327
31	16	0	77	91	3	-2	376	403	5	5	341	346
									5	6	477	450

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
5	7	234	243	8	-8	384	361	11	-3	244	267	1	-14	308	307
5	10	618	603	8	-6	258	262	11	-2	967	944	1	-13	347	369
5	11	823	821	8	-5	170	175	11	-1	942	982	1	-12	214	228
5	12	291	324	8	-4	208	220	11	0	107	108	1	-9	246	245
6	-12	296	301	8	-3	87	80	11	1	255	251	1	-7	549	525
6	-11	335	353	8	-2	132	144	11	2	319	311	1	-6	200	219
6	-10	345	296	8	-1	459	453	11	3	455	452	1	-4	466	443
6	-9	251	209	8	1	80	65	11	4	349	337	1	-3	92	78
6	-8	327	279	8	2	387	371	11	5	145	132	1	-2	1047	1014
6	-7	1024	1034	8	3	118	130	11	7	147	101	1	-1	410	412
6	-6	1005	1002	8	4	1130	1103	11	8	83	83	1	0	1916	2161
6	-5	820	835	8	5	1057	1051	11	9	169	199	1	1	1269	1293
6	-4	94	90	8	6	446	478	12	-9	282	258	1	2	501	403
6	-3	235	209	8	7	138	113	12	-8	689	687	1	3	805	809
6	-2	1019	1023	8	8	102	65	12	-7	466	481	1	4	485	479
6	-1	664	662	8	9	307	311	12	-6	131	119	1	5	1608	1557
6	0	241	237	8	10	597	616	12	-4	456	427	1	6	860	877
6	1	269	277	8	11	352	339	12	-3	774	796	1	7	373	395
6	2	248	261	9	-12	328	332	12	-2	711	712	1	10	83	18
6	3	322	366	9	-11	219	212	12	-1	91	83	1	11	156	125
6	4	1022	960	9	-10	138	126	12	0	195	194	1	12	262	240
6	5	920	933	9	-8	210	204	12	1	312	305	2	-13	72	56
6	6	396	421	9	-6	149	132	12	2	298	302	2	-12	168	156
6	7	219	235	9	-5	97	102	12	3	111	88	2	-10	85	59
6	8	484	485	9	-3	305	331	12	4	101	101	2	-8	301	333
6	9	878	867	9	-2	864	879	12	7	144	124	2	-7	661	692
6	10	1025	1008	9	-1	694	703	12	8	159	162	2	-6	1395	1406
6	11	222	214	9	2	339	321	13	-9	411	426	2	-5	1199	1201
6	12	167	161	9	3	943	961	13	-8	298	284	2	-4	154	157
7	-13	631	651	9	4	894	877	13	-7	145	105	2	-3	1214	1286
7	-12	598	623	9	5	134	132	13	-6	257	255	2	-2	2359	2546
7	-11	259	260	9	7	338	309	13	-5	249	255	2	-1	1841	1949
7	-9	363	390	9	8	336	394	13	-4	328	314	2	0	1612	1718
7	-8	1027	1023	9	9	192	204	13	-1	327	355	2	1	1368	1377
7	-7	886	849	9	10	163	142	13	0	261	239	2	2	59	76
7	-6	353	321	10	-12	93	90	13	4	152	137	2	3	630	604
7	-5	172	177	10	-9	108	132	13	5	165	175	2	4	689	662
7	-4	292	291	10	-8	103	141	13	6	91	97	2	5	870	813
7	-3	381	397	10	-7	172	160	13	7	87	81	2	7	111	87
7	-2	119	109	10	-6	265	278	14	-8	376	375	2	8	251	238
7	-1	302	273	10	-3	496	530	14	-7	428	425	2	10	211	219
7	0	131	163	10	-2	525	560	14	-6	196	174	2	11	169	162
7	2	195	171	10	-1	317	327	14	-3	328	321	2	13	166	158
7	3	665	622	10	0	528	526	14	-2	391	407	2	14	105	116
7	4	439	450	10	1	336	338	14	1	99	103	3	-13	80	85
7	5	252	263	10	2	250	257	14	2	95	74	3	-12	252	247
7	6	429	434	10	3	361	353	14	3	203	191	3	-10	136	116
7	7	259	232	10	4	246	233	14	4	256	273	3	-8	648	642
7	8	340	335	10	5	414	416	14	5	129	134	3	-7	826	863
7	9	512	497	10	6	270	268	15	-7	166	174	3	-6	831	811
7	10	114	99	10	9	177	153	15	-5	115	100	3	-5	307	342
7	11	465	469	10	10	94	82	15	-3	150	131	3	-4	562	523
7	12	297	302	11	-9	154	163	16	-2	110	107	3	-3	197	225
8	-11	208	217	11	-8	111	74	16	-1	232	223	3	-2	636	677
8	-10	241	237	11	-7	542	573	16	0	89	76	3	-1	856	845
8	-9	410	407	11	-6	582	554	16	2	211	213	3	0	582	571
				11	-5	138	151					3	1	193	171

\*\*H = -1\*\*\*\*

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
3	2	1166	1214	5	11	339	339	8	-3	171	54	11	0	172	85
3	3	409	408	5	12	336	337	8	-2	626	639	11	1	99	111
3	4	458	452	5	13	144	135	8	-1	585	603	11	2	108	121
3	5	529	493	6	-13	607	606	8	0	336	338	11	3	190	205
3	6	229	234	6	-12	269	217	8	1	337	338	11	5	282	254
3	7	210	206	6	-11	256	221	8	2	315	330	11	6	372	370
3	11	637	650	6	-10	378	363	8	3	980	1006	11	7	260	255
3	12	521	513	6	-9	477	450	8	4	327	340	11	9	325	313
4	-14	72	58	6	-8	616	593	8	6	370	358	12	-10	89	110
4	-13	111	93	6	-7	103	77	8	7	314	331	12	-9	145	131
4	-12	267	309	6	-6	464	447	8	8	440	408	12	-8	401	391
4	-11	624	631	6	-5	643	616	8	10	126	106	12	-7	763	749
4	-10	112	68	6	-4	227	236	8	11	68	57	12	-6	531	539
4	-8	129	82	6	-2	385	407	9	-9	124	81	12	-5	192	196
4	-7	683	730	6	0	461	467	9	-8	131	104	12	-4	234	242
4	-6	1077	1089	6	1	1100	1097	9	-7	190	140	12	-3	299	305
4	-5	718	768	6	2	177	167	9	-6	417	403	12	-2	668	691
4	-4	418	402	6	3	266	193	9	-5	186	213	12	-1	300	290
4	-3	149	159	6	4	380	381	9	-3	164	128	12	0	111	105
4	-2	459	454	6	5	1363	1364	9	-2	323	311	12	2	108	91
4	-1	775	798	6	6	1346	1297	9	-1	861	885	12	4	413	417
4	0	809	820	6	7	448	449	9	0	766	775	12	5	238	221
4	2	752	743	6	9	238	236	9	1	238	216	12	7	125	107
4	3	452	456	6	10	687	681	9	2	210	165	12	8	298	312
4	4	473	452	6	11	522	533	9	3	224	189	13	-10	80	63
4	5	726	747	6	12	177	185	9	4	676	653	13	-9	383	391
4	6	798	754	7	-13	159	167	9	5	668	667	13	-8	615	600
4	8	431	412	7	-12	522	520	9	6	117	128	13	-7	450	424
4	9	340	348	7	-11	388	416	9	7	137	89	13	-4	145	103
4	10	838	842	7	-10	238	225	9	10	145	163	13	-3	332	360
4	11	711	718	7	-9	188	191	10	-9	103	85	13	-1	88	73
4	12	82	94	7	-8	147	126	10	-8	295	290	13	2	251	263
4	13	96	80	7	-7	433	390	10	-7	766	741	13	3	466	437
5	-13	487	491	7	-6	540	521	10	-6	571	566	13	4	171	165
5	-12	797	810	7	-5	143	138	10	-5	151	126	13	5	231	200
5	-11	286	325	7	-4	307	319	10	-4	330	317	13	6	281	284
5	-10	384	415	7	-2	272	268	10	-3	494	511	13	7	151	160
5	-9	149	161	7	-1	863	906	10	-2	1098	1136	14	-8	112	116
5	-8	933	905	7	0	879	876	10	-1	751	789	14	-7	100	133
5	-7	1478	1461	7	1	497	506	10	0	150	128	14	-6	326	345
5	-6	1088	1106	7	3	718	716	10	1	162	195	14	-5	202	200
5	-5	340	329	7	4	1636	1634	10	2	273	302	14	-3	123	84
5	-4	231	262	7	5	1476	1468	10	3	460	471	14	-1	116	127
5	-3	492	529	7	6	458	430	10	4	386	360	14	0	163	165
5	-2	729	728	7	7	375	376	10	5	131	146	14	2	131	118
5	-1	304	306	7	8	312	284	10	6	139	137	14	3	145	149
5	1	332	350	7	9	653	638	10	9	93	113	14	4	515	505
5	2	316	324	7	10	466	501	11	-11	113	109	14	5	453	451
5	3	548	569	7	11	85	78	11	-10	193	233	14	6	145	136
5	4	694	701	7	12	135	129	11	-9	401	366	15	-7	187	228
5	5	515	513	8	-13	493	508	11	-8	426	403	15	-6	140	144
5	6	320	302	8	-12	430	439	11	-7	123	120	15	-3	131	99
5	7	574	560	8	-11	179	145	11	-6	256	287	15	-2	211	249
5	8	344	334	8	-9	285	280	11	-5	388	353	15	-1	131	140
5	9	445	448	8	-8	144	153	11	-4	164	158	15	0	111	111
5	10	213	196	8	-6	122	132	11	-3	253	236	15	2	261	273
5				8	-5	111	47	11	-1	574	587	15	3	531	531

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -1****				2	0	1294	1397	4	11	707	712	7	-3	553	566
15	4	394	375	2	1	1160	1121	4	12	430	458	7	-2	442	426
16	-4	213	229	2	2	1079	1027	4	13	82	64	7	-1	934	937
16	-3	196	179	2	4	106	107	5	-14	187	199	7	0	1372	1421
16	-1	223	223	2	5	548	513	5	-13	218	238	7	1	1053	1095
16	0	179	190	2	6	420	436	5	-12	304	320	7	2	422	412
16	1	131	130	2	7	100	33	5	-11	894	896	7	3	85	91
16	2	110	100	2	10	482	516	5	-10	393	379	7	4	626	669
**H = 0****				2	11	829	853	5	-9	149	197	7	5	976	955
0	1	1810	1813	2	12	600	594	5	-7	492	493	7	6	870	830
0	2	125	95	2	13	121	134	5	-6	644	617	7	7	186	208
0	3	373	368	2	14	63	73	5	-5	180	172	7	8	166	172
0	4	1266	1228	3	-13	95	81	5	-4	122	122	7	9	178	200
0	5	1563	1545	3	-12	460	457	5	-3	187	198	7	10	124	129
0	6	957	984	3	-11	789	790	5	-2	72	55	7	12	95	107
0	7	211	196	3	-10	315	321	5	-1	824	838	8	-12	238	242
0	8	488	540	3	-8	115	49	5	0	1046	1082	8	-11	108	98
0	10	148	163	3	-7	931	857	5	1	894	964	8	-10	93	121
0	11	281	316	3	-6	1214	1199	5	2	201	178	8	-7	447	426
0	12	262	260	3	-5	1076	1067	5	3	322	358	8	-6	413	443
0	13	148	134	3	-4	288	322	5	4	1212	1183	8	-5	363	342
0	14	148	148	3	-1	1391	1419	5	5	1596	1589	8	-4	385	364
1	-14	82	54	3	0	776	814	5	6	1181	1118	8	-3	329	302
1	-13	141	147	3	1	1067	1027	5	8	221	217	8	-2	1004	1048
1	-12	190	168	3	2	750	727	5	9	442	426	8	-1	1692	1767
1	-10	244	259	3	3	495	469	5	10	658	656	8	0	1015	1059
1	-9	143	171	3	4	116	111	5	11	480	476	8	2	108	111
1	-7	874	873	3	5	542	480	5	13	99	108	8	3	596	603
1	-6	1160	1175	3	6	273	282	6	-13	548	533	8	4	721	746
1	-5	535	548	3	8	293	283	6	-12	757	745	8	5	720	746
1	-4	226	224	3	9	231	183	6	-11	239	244	8	6	136	98
1	-3	114	83	3	10	382	365	6	-9	106	124	8	7	197	155
1	-2	268	238	3	11	170	179	6	-8	353	355	8	10	231	186
1	-1	1631	1800	3	12	215	220	6	-7	388	390	9	-10	207	228
1	0	723	733	3	13	165	178	6	-5	166	161	9	-9	160	121
1	1	768	688	4	-14	126	135	6	-4	195	180	9	-8	266	282
1	2	241	211	4	-13	421	394	6	-3	254	249	9	-7	703	673
1	3	226	207	4	-12	591	585	6	-2	1413	1430	9	-6	136	119
1	4	547	535	4	-11	85	49	6	-1	344	370	9	-5	331	336
1	6	223	193	4	-10	132	207	6	0	83	83	9	-4	244	265
1	8	126	71	4	-9	144	132	6	1	311	305	9	-3	475	457
1	9	284	261	4	-8	661	648	6	2	613	646	9	-2	615	649
1	10	170	143	4	-7	524	525	6	3	889	920	9	-1	341	357
1	11	159	180	4	-6	265	237	6	4	976	985	9	0	463	475
1	12	475	481	4	-5	554	540	6	5	433	451	9	1	288	269
1	13	354	368	4	-4	232	234	6	6	512	500	9	2	323	292
1	14	246	242	4	-3	521	522	6	7	568	533	9	3	219	231
2	-11	189	172	4	-1	441	457	6	8	115	73	9	9	182	157
2	-10	197	206	4	0	200	229	6	9	111	147	9	10	147	103
2	-9	151	181	4	1	836	831	6	11	115	113	9	11	387	375
2	-8	268	273	4	2	509	529	7	-13	404	414	10	-12	114	105
2	-6	486	539	4	3	359	349	7	-12	140	140	10	-11	185	188
2	-5	1298	1354	4	5	968	916	7	-11	207	193	10	-10	179	162
2	-4	1389	1406	4	6	1045	1044	7	-10	338	326	10	-9	140	125
2	-3	246	248	4	7	786	779	7	-9	225	225	10	-7	375	349
2	-2	1224	1203	4	8	117	128	7	-7	216	234	10	-6	742	732
2	-1	626	614	4	10	382	360	7	-5	211	209	10	-5	529	523



Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	0****													
10	-2	552	558	14	-9	136	167	1	-8	116	115	3	-4	546	514
10	-1	600	603	14	-8	98	72	1	-7	318	341	3	-3	661	622
10	0	503	523	14	-4	121	113	1	-6	1493	1486	3	-2	1080	1043
10	1	353	364	14	-3	127	105	1	-5	2034	2001	3	-1	481	470
10	3	161	135	14	-2	411	426	1	-4	1390	1317	3	0	1418	1456
10	4	320	310	14	2	229	229	1	-3	90	112	3	1	531	531
10	5	250	232	14	3	412	425	1	-2	155	117	3	2	1082	1006
10	6	136	130	14	4	148	134	1	-1	1073	990	3	3	217	172
10	9	436	450	14	5	243	255	1	0	1937	2006	3	4	413	388
10	10	612	618	14	6	242	236	1	1	621	583	3	5	1170	1130
11	-11	127	140	15	-7	92	68	1	2	148	122	3	6	1267	1247
11	-9	213	244	15	-4	123	124	1	4	439	415	3	7	292	303
11	-8	706	673	15	-2	382	388	1	5	545	505	3	8	129	92
11	-7	745	778	15	-1	431	425	1	6	783	751	3	10	526	527
11	-6	411	404	15	0	404	435	1	8	158	153	3	11	739	732
11	-5	93	58	15	1	89	72	1	9	142	159	3	12	378	379
11	-4	353	386	15	3	241	222	1	10	581	573	3	13	143	140
11	-3	257	275	15	4	466	467	1	11	642	638	4	-13	181	186
11	-2	341	323	15	5	312	323	1	12	97	73	4	-12	624	645
11	1	173	196	16	-4	105	84	1	13	158	176	4	-11	864	871
11	2	206	218	16	-3	386	389	1	14	249	263	4	-10	323	303
11	3	542	542	16	-2	420	428	2	-13	190	192	4	-9	103	107
11	4	392	398	16	-1	189	199	2	-12	520	562	4	-8	303	305
11	6	327	324	16	2	149	133	2	-11	500	473	4	-7	504	525
11	7	181	173		**H =	1****		2	-10	203	191	4	-6	845	816
11	8	324	327	0	-14	101	138	2	-9	138	130	4	-5	204	191
11	9	227	236	0	-13	120	103	2	-8	562	619	4	-4	365	330
12	-11	171	168	0	-12	176	173	2	-7	1086	1116	4	-3	175	171
12	-10	240	218	0	-11	236	268	2	-6	1138	1150	4	-2	642	659
12	-9	296	297	0	-9	266	263	2	-5	102	59	4	-1	747	783
12	-8	335	302	0	-8	298	288	2	-4	398	412	4	0	244	232
12	-6	340	293	0	-7	647	673	2	-3	482	435	4	1	262	257
12	-5	241	285	0	-6	377	395	2	-2	1198	1126	4	2	315	330
12	-3	137	150	0	-5	1480	1443	2	-1	408	417	4	3	796	773
12	-2	252	260	0	-4	2085	2078	2	0	191	174	4	4	623	630
12	-1	88	88	0	-3	2739	2826	2	1	503	467	4	5	754	728
12	0	172	155	0	-2	504	484	2	2	626	534	4	6	92	66
12	1	128	116	0	-1	481	423	2	3	561	525	4	7	411	426
12	2	108	91	0	0	1077	1104	2	4	132	106	4	8	126	145
12	4	331	336	0	1	1257	1348	2	5	188	198	4	9	247	198
12	5	689	684	0	2	869	849	2	6	109	133	4	10	259	249
12	6	427	432	0	3	382	334	2	7	981	993	4	12	124	147
12	7	130	128	0	4	152	135	2	8	308	308	5	-14	199	214
12	8	85	113	0	5	482	494	2	9	391	376	5	-13	467	452
13	-10	148	136	0	6	197	188	2	10	115	127	5	-12	386	411
13	-8	225	225	0	7	401	370	2	11	477	473	5	-11	180	177
13	-7	253	216	0	8	294	324	2	12	655	675	5	-10	133	148
13	-6	284	253	0	9	199	198	2	13	425	416	5	-9	133	118
13	-2	334	371	0	10	205	219	3	-14	99	108	5	-5	107	76
13	-1	564	557	0	11	787	745	3	-13	300	300	5	-4	361	352
13	0	154	170	0	12	830	831	3	-11	376	348	5	-3	602	587
13	2	179	170	0	13	414	432	3	-10	353	336	5	-2	823	867
13	3	497	492	0	14	118	106	3	-9	222	209	5	-1	242	246
13	4	825	834	1	-13	89	93	3	-8	345	344	5	0	641	673
13	5	458	436	1	-11	484	482	3	-7	232	239	5	1	1691	1713
13	7	108	96	1	-10	582	601	3	-6	291	308	5	2	1215	1198
				1	-9	422	400	3	-5	546	530	5	3	449	426



Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
		**H =	1****	8	-5	794	792	11	-2	135	133	15	2	94	109
5	4	410	342	8	-4	414	379	11	-1	529	534	15	3	117	126
5	5	799	760	8	-3	211	237	11	0	558	563	15	5	80	82
5	6	1269	1244	8	-2	246	251	11	1	151	129	16	-5	112	120
5	7	543	541	8	-1	608	634	11	3	364	391	16	-2	308	317
5	9	171	152	8	0	1055	1097	11	4	887	839	16	-1	214	220
5	10	238	245	8	1	402	427	11	5	959	925	16	0	204	204
5	11	160	165	8	2	370	375	11	6	233	260			**H =	2****
5	12	149	131	8	3	253	251	11	7	154	156	0	-14	101	99
5	13	80	98	8	4	188	170	11	9	437	422	0	-12	391	402
6	-12	194	211	8	5	218	176	12	-11	101	93	0	-11	686	671
6	-11	319	315	8	6	115	80	12	-10	88	96	0	-10	551	560
6	-10	266	288	8	8	176	176	12	-9	203	167	0	-9	114	119
6	-8	161	212	8	9	127	128	12	-8	281	300	0	-8	607	593
6	-6	753	701	8	10	349	373	12	-7	191	181	0	-7	779	821
6	-5	912	873	8	11	484	483	12	-5	212	225	0	-6	1396	1472
6	-4	316	264	9	-12	324	308	12	-3	138	111	0	-5	2152	2110
6	-3	263	214	9	-11	173	198	12	-2	568	572	0	-4	540	538
6	-2	570	581	9	-10	146	160	12	-1	430	447	0	-3	915	898
6	-1	1891	2005	9	-8	240	257	12	1	294	324	0	-2	238	261
6	0	2088	2225	9	-7	768	766	12	2	323	326	0	-1	813	792
6	1	981	997	9	-6	991	995	12	3	480	474	0	0	394	435
6	2	162	171	9	-5	590	631	12	4	447	445	0	1	555	560
6	3	855	822	9	-4	111	85	12	5	220	254	0	2	1101	1107
6	4	1043	990	9	-2	626	661	12	6	419	389	0	3	787	808
6	5	1071	1025	9	-1	848	838	12	7	118	96	0	5	657	612
6	6	433	431	9	0	345	342	12	8	184	184	0	6	160	141
6	7	138	143	9	1	345	336	13	-10	158	161	0	7	650	647
6	8	159	181	9	4	259	276	13	-9	143	120	0	8	813	786
6	9	151	120	9	5	413	417	13	-7	90	62	0	9	444	423
6	11	165	151	9	6	159	128	13	-3	212	207	0	10	399	413
7	-13	197	202	9	7	142	120	13	-2	150	136	0	12	601	588
7	-9	386	398	9	8	148	151	13	-1	438	436	0	13	564	569
7	-8	422	432	9	9	325	308	13	0	590	585	0	14	338	360
7	-7	857	843	9	10	386	399	13	1	334	324	1	-13	336	337
7	-6	734	727	10	-12	243	241	13	2	188	198	1	-12	449	441
7	-4	140	153	10	-10	134	120	13	4	376	362	1	-11	90	62
7	-3	434	446	10	-9	380	345	13	5	746	732	1	-10	362	376
7	-2	1565	1652	10	-8	525	483	13	6	390	385	1	-9	623	592
7	-1	1362	1393	10	-7	271	267	14	-7	195	201	1	-8	692	656
7	0	184	166	10	-5	415	423	14	-6	203	159	1	-7	704	699
7	1	199	231	10	-3	292	327	14	-4	100	97	1	-6	359	354
7	2	487	499	10	-2	137	128	14	-3	110	72	1	-5	1063	1068
7	3	508	494	10	-1	244	206	14	-2	608	627	1	-4	1337	1292
7	4	353	320	10	1	415	407	14	-1	714	712	1	-3	220	222
7	5	121	100	10	3	146	136	14	0	375	385	1	-2	339	311
7	6	210	196	10	4	153	151	14	2	140	149	1	-1	142	137
7	9	141	164	10	5	708	710	14	3	295	295	1	0	303	283
7	10	139	149	10	6	643	628	14	4	475	483	1	1	820	799
7	11	141	133	10	7	143	101	14	5	262	238	1	2	375	373
7	12	352	360	10	10	538	539	15	-7	176	173	1	3	370	373
8	-12	123	103	11	-11	375	364	15	-6	118	117	1	4	248	211
8	-10	103	61	11	-10	171	177	15	-5	134	147	1	5	277	263
8	-9	100	137	11	-8	190	182	15	-3	451	443	1	6	1132	1158
8	-8	236	228	11	-7	429	421	15	-2	265	253	1	7	1465	1450
8	-7	126	120	11	-6	488	524	15	0	205	206	1	8	469	468
8	-6	638	617	11	-4	130	149	15	1	217	229	1	10	217	230

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H =		2****													
1	11	872	834	4	-14	66	77	6	1	959	964	9	-2	200	165
1	12	704	711	4	-13	220	190	6	2	499	501	9	-1	222	203
1	13	396	384	4	-12	93	65	6	3	102	91	9	0	94	118
2	-14	68	87	4	-11	339	322	6	4	613	579	9	1	212	233
2	-13	115	106	4	-10	165	141	6	5	307	318	9	2	124	147
2	-12	377	359	4	-8	106	147	6	8	167	154	9	3	108	124
2	-11	867	878	4	-7	133	142	6	10	250	252	9	4	258	274
2	-10	633	655	4	-6	379	337	6	11	571	576	9	5	867	858
2	-9	465	454	4	-5	607	633	6	12	610	653	9	6	741	695
2	-7	114	131	4	-4	657	621	7	-11	474	499	9	7	194	182
2	-6	823	826	4	-3	441	423	7	-10	344	288	9	9	160	188
2	-5	774	763	4	-2	329	341	7	-8	107	113	9	9	160	188
2	-4	721	720	4	-1	521	511	7	-7	591	595	9	10	479	491
2	-3	388	376	4	0	2076	2258	7	-6	1553	1526	9	11	476	477
2	-2	170	174	4	1	1302	1325	7	-5	1346	1357	10	-12	545	542
2	-1	665	634	4	2	923	887	7	-4	442	432	10	-11	316	322
2	0	1194	1259	4	4	584	594	7	-3	113	142	10	-8	220	248
2	1	1079	1082	4	5	1395	1363	7	-2	276	337	10	-7	363	335
2	2	1561	1511	4	6	1180	1168	7	-1	1202	1226	10	-6	337	325
2	3	210	181	4	7	416	403	7	0	1213	1263	10	-3	101	100
2	4	547	536	4	8	96	73	7	1	405	397	10	-2	439	473
2	5	969	968	4	11	159	136	7	2	170	165	10	-1	414	429
2	6	1123	1113	5	-14	77	80	7	3	178	156	10	0	305	321
2	7	275	228	5	-13	169	184	7	5	111	91	10	1	238	242
2	8	341	348	5	-12	311	330	7	6	328	343	10	2	347	348
2	9	165	179	5	-11	193	182	7	7	114	114	10	3	225	247
2	10	348	383	5	-7	399	362	7	9	239	230	10	4	556	536
2	11	422	436	5	-6	1230	1211	7	10	471	456	10	5	398	390
3	-14	77	95	5	-5	659	689	7	11	440	431	10	6	182	167
3	-13	299	299	5	-4	126	122	8	-13	191	192	10	7	434	438
3	-12	595	620	5	-3	601	617	8	-12	453	462	10	9	169	151
3	-11	451	417	5	-2	1419	1406	8	-11	163	138	11	-11	113	126
3	-10	127	134	5	-1	1595	1660	8	-8	385	377	11	-10	197	186
3	-9	183	178	5	0	477	527	8	-7	875	825	11	-9	141	148
3	-8	168	164	5	1	283	282	8	-6	813	798	11	-8	124	117
3	-7	442	435	5	2	302	333	8	-4	157	155	11	-6	151	116
3	-6	560	537	5	3	330	359	8	-3	385	402	11	-5	186	205
3	-5	494	493	5	4	228	248	8	-2	417	407	11	-4	255	208
3	-4	563	540	5	5	298	291	8	-1	343	372	11	-3	207	178
3	-3	542	530	5	7	282	293	8	0	103	109	11	-2	105	119
3	-2	678	619	5	8	98	69	8	1	305	273	11	-1	138	102
3	-1	1069	951	5	9	349	353	8	2	419	398	11	0	610	612
3	0	1290	1277	5	11	106	83	8	3	95	48	11	1	683	712
3	1	1067	965	5	12	268	274	8	4	202	179	11	2	203	203
3	2	817	734	5	13	279	283	8	6	298	285	11	3	125	137
3	3	182	177	6	-13	129	132	8	7	491	483	11	4	228	203
3	4	452	439	6	-12	202	209	8	8	203	210	11	5	777	793
3	5	257	249	6	-10	151	186	8	9	205	213	11	6	678	642
3	6	976	949	6	-9	172	172	8	11	410	431	11	8	113	125
3	7	868	847	6	-8	345	296	9	-11	236	248	12	-11	184	201
3	8	315	281	6	-7	782	803	9	-10	297	322	12	-9	91	92
3	9	144	138	6	-5	863	832	9	-9	400	399	12	-7	154	178
3	10	175	196	6	-4	1027	1027	9	-8	319	352	12	-6	356	351
3	11	164	153	6	-3	679	710	9	-6	593	583	12	-5	378	411
3	12	288	293	6	-2	748	731	9	-5	616	607	12	-4	101	103
3	13	83	85	6	-1	99	69	9	-4	398	427	12	-2	569	565
3				6	0	1585	1613	9	-3	366	335	12	-1	883	877
												12	0	695	707

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 2****				0	1	140	117	2	8	465	459	5	0	1230	1283
12	1	144	141	0	2	1248	1294	2	9	206	175	5	1	680	678
12	2	243	228	0	4	837	830	2	11	302	320	5	2	387	363
12	3	309	321	0	5	900	933	2	12	265	266	5	4	123	141
12	4	501	482	0	6	1464	1426	3	-12	285	287	5	5	108	61
12	5	545	517	0	7	696	678	3	-11	458	452	5	6	450	407
12	7	137	165	0	8	199	215	3	-10	366	375	5	9	235	231
13	-10	71	84	0	9	220	190	3	-9	236	238	5	10	361	355
13	-8	140	141	0	10	448	441	3	-8	266	251	5	11	501	494
13	-7	396	400	0	11	640	656	3	-7	228	228	5	12	250	252
13	-6	378	395	0	12	237	239	3	-6	431	475	6	-13	72	56
13	-4	174	183	0	13	131	120	3	-5	572	552	6	-12	298	332
13	-3	467	495	1	-13	133	153	3	-4	125	102	6	-11	655	642
13	-2	592	585	1	-12	741	764	3	-2	127	108	6	-10	418	413
13	-1	508	529	1	-11	935	949	3	-1	315	289	6	-9	315	331
13	0	108	102	1	-10	527	541	3	0	2031	2090	6	-8	485	464
13	1	395	409	1	-8	478	483	3	1	1556	1643	6	-7	1093	1081
13	2	384	372	1	-7	635	645	3	2	568	575	6	-6	1550	1568
13	3	265	276	1	-6	449	441	3	3	321	310	6	-5	722	696
13	4	141	145	1	-5	403	394	3	4	162	108	6	-4	740	673
13	5	113	79	1	-4	462	412	3	5	1029	991	6	-3	747	738
13	6	176	173	1	-3	327	296	3	6	528	531	6	-2	529	537
14	-9	87	64	1	-2	288	274	3	7	120	117	6	-1	668	651
14	-8	243	224	1	-1	349	367	3	11	133	109	6	0	111	57
14	-6	341	333	1	0	1045	1056	3	13	149	165	6	1	402	410
14	-5	259	272	1	1	1578	1602	4	-13	108	99	6	2	550	573
14	-4	248	233	1	2	1021	1030	4	-12	218	235	6	3	121	146
14	-3	219	210	1	3	1433	1446	4	-11	204	223	6	4	118	75
14	-1	389	423	1	4	743	759	4	-9	152	124	6	5	260	240
14	0	499	488	1	5	843	823	4	-8	277	293	6	7	301	302
14	1	283	297	1	7	951	944	4	-7	507	520	6	8	404	413
14	2	128	98	1	8	921	864	4	-6	603	571	6	9	383	404
14	4	246	250	1	9	350	347	4	-5	712	665	6	10	108	133
14	5	129	114	1	10	277	269	4	-4	521	497	6	11	120	145
15	-7	476	448	1	11	118	142	4	-3	514	513	6	12	472	479
15	-6	366	352	1	12	349	351	4	-2	846	821	7	-13	281	284
15	-5	111	138	1	13	336	322	4	-1	942	860	7	-12	405	406
15	-3	257	283	2	-14	138	147	4	0	1232	1157	7	-10	530	547
15	-2	434	425	2	-13	379	394	4	1	1535	1455	7	-9	241	237
15	-1	265	273	2	-12	392	402	4	2	1304	1232	7	-8	347	335
15	4	87	82	2	-10	221	241	4	5	159	165	7	-7	693	714
16	-5	171	178	2	-9	299	284	4	6	602	617	7	-5	756	769
16	-3	145	159	2	-8	149	150	4	7	197	189	7	-4	803	763
**H = 3****				2	-7	538	512	4	9	108	103	7	-3	396	389
0	-14	103	117	2	-5	406	391	4	11	373	377	7	-2	283	311
0	-13	235	247	2	-4	185	179	4	12	437	445	7	-1	169	174
0	-11	704	733	2	-3	131	116	4	13	275	272	7	0	123	140
0	-10	964	949	2	-2	665	644	5	-13	64	60	7	1	171	166
0	-9	902	901	2	-1	1213	1169	5	-11	300	290	7	2	173	159
0	-8	620	603	2	0	529	562	5	-10	362	330	7	4	111	102
0	-6	880	853	2	1	1360	1425	5	-9	310	332	7	5	421	404
0	-5	1523	1491	2	2	707	711	5	-6	1148	1128	7	6	841	832
0	-4	550	527	2	3	154	117	5	-5	1562	1580	7	7	701	687
0	-3	193	185	2	4	105	106	5	-4	773	755	7	8	232	243
0	-2	498	489	2	5	329	352	5	-3	147	133	7	9	91	60
0	-1	1155	1142	2	6	1464	1450	5	-2	245	213	7	10	424	417
0	0	269	279	2	7	1022	1063	5	-1	992	980	7	11	639	666

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	3****		10	5	903	872	15	-6	365	379	2	-8	226	236
7	12	471	491	10	6	396	386	15	-5	162	179	2	-7	180	143
8	-12	349	349	11	-11	105	104	15	-4	106	103	2	-6	217	223
8	-11	583	607	11	-9	134	146	15	4	221	210	2	-5	482	472
8	-10	546	532	11	-8	206	209	16	-2	115	124	2	-4	139	129
8	-9	308	309	11	-7	278	240	16	-1	211	224	2	-3	727	701
8	-7	305	291	11	-6	538	517	16	2	107	113	2	-2	274	262
8	-6	1113	1127	11	-5	122	137		**H =	4****		2	-1	183	200
8	-5	458	448	11	-3	307	323	0	-13	269	275	2	0	1012	1019
8	-4	181	180	11	-2	777	770	0	-12	627	645	2	1	801	798
8	-3	206	177	11	-1	841	859	0	-11	505	521	2	2	1191	1198
8	-2	465	435	11	0	248	205	0	-9	495	485	2	3	1025	1027
8	0	375	353	11	1	426	411	0	-8	381	366	2	4	619	630
8	1	238	240	11	2	399	414	0	-6	91	65	2	5	579	535
8	3	235	226	11	3	230	220	0	-5	380	345	2	7	444	449
8	4	563	567	11	4	419	397	0	-4	162	175	2	8	475	459
8	5	770	776	11	5	148	141	0	-3	352	346	2	10	127	101
8	6	532	503	11	6	246	239	0	-2	358	366	2	11	141	168
8	7	153	133	11	7	98	101	0	-1	404	405	2	12	182	176
8	8	174	184	11	9	106	91	0	0	92	91	2	13	209	202
8	9	387	380	12	-9	158	135	0	1	1376	1386	3	-13	97	118
8	10	354	367	12	-8	232	245	0	2	1599	1673	3	-12	143	155
8	11	182	182	12	-7	139	139	0	3	1177	1182	3	-11	174	144
9	-12	527	524	12	-6	126	92	0	5	172	169	3	-10	166	171
9	-11	158	163	12	-5	466	471	0	6	1172	1147	3	-9	253	290
9	-9	263	265	12	-4	330	318	0	7	1594	1580	3	-7	192	164
9	-8	218	167	12	-3	306	327	0	8	735	731	3	-6	151	125
9	-7	302	320	12	-2	238	240	0	10	124	92	3	-5	1084	1040
9	-6	422	401	12	-1	231	247	0	11	208	226	3	-4	1171	1150
9	-4	108	44	12	0	664	661	0	12	390	374	3	-3	391	375
9	-2	245	264	12	1	483	486	0	13	198	203	3	-2	187	183
9	-1	291	312	12	2	95	73	1	-13	209	224	3	-1	676	675
9	0	368	386	12	4	106	130	1	-12	98	88	3	0	960	1004
9	1	352	328	12	5	153	157	1	-11	534	568	3	1	1516	1619
9	2	317	296	13	-7	431	408	1	-10	662	641	3	2	1113	1125
9	3	219	212	13	-6	663	676	1	-9	308	295	3	3	197	177
9	4	212	198	13	-5	364	350	1	-8	152	164	3	4	160	147
9	5	152	127	13	-4	103	69	1	-6	95	61	3	5	185	176
9	6	739	708	13	-3	121	127	1	-5	101	68	3	6	241	263
9	7	467	476	13	-2	386	396	1	-4	720	669	3	7	321	287
9	8	277	268	13	-1	631	636	1	-3	96	120	3	9	95	101
9	9	121	142	13	0	444	451	1	-2	121	109	3	10	103	115
10	-12	94	103	13	1	106	111	1	-1	945	965	3	11	346	362
10	-11	245	238	13	3	281	270	1	0	1808	1882	3	12	300	283
10	-10	131	163	13	6	86	95	1	1	785	807	3	13	106	103
10	-7	171	196	14	-8	379	383	1	2	768	776	4	-12	198	190
10	-6	93	61	14	-7	600	615	1	3	413	417	4	-11	481	494
10	-5	398	439	14	-6	228	194	1	4	428	446	4	-10	438	455
10	-4	240	230	14	-4	158	170	1	5	786	779	4	-8	300	314
10	-3	145	152	14	-3	339	360	1	6	987	981	4	-7	563	578
10	-2	386	405	14	-2	360	355	1	7	344	336	4	-6	1310	1336
10	-1	828	836	14	-1	158	137	1	8	258	260	4	-5	1290	1273
10	0	1037	1042	14	0	119	124	1	10	230	226	4	-4	117	121
10	1	588	579	14	1	166	179	1	11	100	94	4	-3	423	400
10	2	107	144	14	4	143	144	2	-12	306	290	4	-2	146	129
10	3	139	109	14	6	217	243	2	-11	325	319	4	-1	1229	1188
10	4	517	523	15	-7	118	105	2	-10	256	246	4	0	971	1007

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 4****															
4	2	243	257	7	-11	755	776	9	6	188	197	13	0	361	380
4	3	251	241	7	-10	454	477	9	8	122	113	13	4	111	118
4	4	122	120	7	-9	105	110	9	10	121	110	13	5	306	310
4	5	396	335	7	-8	306	310	10	-12	79	93	13	6	520	529
4	7	281	251	7	-7	732	744	10	-11	79	78	13	7	199	183
4	8	486	452	7	-6	687	627	10	-10	126	132	14	-8	77	91
4	9	199	185	7	-5	101	102	10	-8	112	141	14	-7	444	451
4	10	114	123	7	-4	135	165	10	-7	370	356	14	-6	517	491
4	11	131	147	7	-3	101	46	10	-6	112	94	14	-5	239	246
4	12	291	286	7	-2	344	307	10	-5	445	416	14	-3	104	108
5	-13	154	124	7	-1	329	323	10	-4	275	264	14	-2	249	243
5	-12	379	397	7	0	109	66	10	-3	259	249	14	-1	126	108
5	-11	315	352	7	1	156	145	10	-2	288	283	14	3	102	63
5	-9	395	377	7	2	327	335	10	-1	154	159	14	4	243	245
5	-8	426	462	7	3	375	381	10	0	281	274	14	5	352	337
5	-7	653	633	7	4	556	543	10	1	760	771	15	-7	237	251
5	-6	740	708	7	5	321	313	10	2	220	200	15	-2	87	50
5	-5	291	290	7	6	310	307	10	4	131	91	15	1	211	212
5	-4	1046	995	7	7	648	629	10	5	176	160	15	2	90	95
5	-3	343	362	7	8	553	565	10	6	238	235	15	3	177	169
5	-2	467	435	7	9	259	264	11	-11	149	178	16	-2	119	120
5	0	442	405	7	10	166	137	11	-10	152	143	16	-1	381	390
5	1	161	156	7	11	108	106	11	-9	276	280	16	0	431	431
5	2	404	421	8	-12	249	241	11	-7	251	250	**H = 5****			
5	4	348	331	8	-11	184	197	11	-6	967	948	0	-12	355	371
5	5	399	420	8	-10	270	258	11	-5	689	665	0	-11	564	572
5	6	833	835	8	-9	325	339	11	-4	231	283	0	-10	376	352
5	7	837	833	8	-8	161	161	11	-3	223	235	0	-9	110	123
5	8	382	382	8	-6	112	125	11	-2	520	540	0	-8	161	168
5	10	185	192	8	-2	142	146	11	-1	727	709	0	-6	136	147
5	11	553	544	8	-1	94	110	11	0	806	813	0	-5	787	782
5	12	688	717	8	0	571	607	11	1	278	273	0	-4	446	445
6	-12	114	146	8	1	824	872	11	2	345	353	0	-3	165	151
6	-11	694	664	8	2	601	571	11	6	216	190	0	-2	635	650
6	-10	870	855	8	3	333	309	11	9	225	215	0	-1	1315	1326
6	-9	331	353	8	4	108	96	12	-9	96	94	0	0	1467	1527
6	-7	269	270	8	5	682	679	12	-8	326	359	0	1	677	702
6	-6	788	821	8	6	996	970	12	-7	667	672	0	2	175	201
6	-5	1004	971	8	7	495	493	12	-6	608	577	0	3	1315	1354
6	-4	415	419	8	8	199	199	12	-5	186	216	0	4	511	528
6	-3	332	316	8	10	224	239	12	-4	165	186	0	5	629	658
6	-1	580	576	8	11	312	332	12	-3	464	482	0	6	292	293
6	1	315	338	9	-12	301	308	12	-2	422	399	0	7	557	561
6	2	614	518	9	-11	369	349	12	-1	351	329	0	8	589	584
6	3	395	358	9	-10	226	236	12	1	150	168	0	9	205	196
6	4	537	516	9	-7	108	116	12	3	108	128	0	10	108	75
6	5	1045	1020	9	-6	234	236	12	5	138	116	0	12	170	152
6	6	1047	1019	9	-5	307	286	12	7	204	192	0	13	165	153
6	7	272	299	9	-3	163	187	12	8	168	175	1	-13	111	130
6	8	164	149	9	-2	209	197	13	-9	131	139	1	-12	146	157
6	9	362	353	9	-1	736	740	13	-8	372	350	1	-11	123	131
6	10	476	501	9	0	895	938	13	-7	238	229	1	-7	351	358
6	11	481	484	9	1	205	224	13	-6	242	240	1	-5	271	284
6	12	157	157	9	2	265	282	13	-5	331	320	1	-4	548	594
7	-13	322	317	9	3	341	336	13	-4	356	343	1	-3	764	779
7	-12	580	590	9	4	457	470	13	-3	245	242	1	-2	471	515
				9	5	721	721	13	-1	207	200	1	-1	256	257

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	5****		3	11	206	217	6	1	1455	1494	9	7	105	71
1	0	267	281	3	12	532	546	6	2	668	687	9	9	87	100
1	1	1190	1235	4	-13	140	135	6	3	259	239	9	10	109	109
1	2	1413	1481	4	-11	406	450	6	5	323	313	10	-11	197	203
1	3	460	513	4	-10	764	782	6	6	1147	1150	10	-10	153	164
1	4	289	266	4	-9	525	520	6	7	901	908	10	-7	493	482
1	5	89	75	4	-6	206	207	6	8	303	294	10	-6	1016	1017
1	6	357	371	4	-5	1367	1323	6	10	246	239	10	-5	648	631
1	7	677	681	4	-4	1238	1221	6	11	279	279	10	-3	149	163
1	8	146	150	4	-3	222	256	7	-13	98	98	10	-2	420	425
1	9	260	236	4	-2	121	110	7	-12	237	248	10	-1	589	588
1	10	133	155	4	-1	318	295	7	-11	534	533	10	0	736	748
1	11	218	203	4	0	140	140	7	-10	592	625	10	1	101	84
1	12	306	318	4	2	211	172	7	-9	179	130	10	2	348	322
1	13	315	322	4	3	513	460	7	-6	205	220	10	7	186	197
2	-13	121	114	4	5	300	276	7	-4	224	208	10	8	176	193
2	-11	130	138	4	6	664	666	7	-3	120	135	10	9	156	156
2	-10	209	191	4	7	592	558	7	-1	575	528	11	-11	62	20
2	-9	151	98	4	9	244	246	7	0	1020	959	11	-10	240	240
2	-6	856	846	4	10	233	230	7	1	996	939	11	-9	262	271
2	-5	1186	1166	4	11	415	396	7	2	339	323	11	-8	165	156
2	-4	1384	1388	4	12	442	443	7	4	403	380	11	-7	326	323
2	-3	369	357	5	-13	121	126	7	5	1302	1300	11	-6	112	81
2	-2	169	155	5	-12	459	477	7	6	705	677	11	-5	394	402
2	-1	1040	1038	5	-11	953	976	7	8	90	86	11	-4	333	323
2	0	1273	1286	5	-10	737	735	7	9	214	217	11	-3	110	99
2	1	1686	1724	5	-8	320	314	7	10	229	240	11	-2	93	48
2	2	615	613	5	-7	549	505	7	11	165	166	11	-1	97	107
2	3	166	156	5	-6	772	778	8	-12	323	324	11	1	100	91
2	5	269	268	5	-5	731	709	8	-11	358	364	11	3	173	166
2	6	276	242	5	-4	239	210	8	-7	166	175	11	5	176	165
2	7	224	212	5	-3	412	391	8	-6	285	292	11	6	425	407
2	8	100	80	5	0	165	109	8	-5	175	172	11	7	278	310
2	9	120	120	5	1	743	790	8	-3	270	255	11	8	120	114
2	11	234	213	5	2	569	535	8	-2	413	405	12	-10	278	289
2	12	133	118	5	3	618	630	8	-1	736	699	12	-9	91	88
3	-12	244	281	5	4	435	440	8	0	306	335	12	-7	265	244
3	-11	323	291	5	5	664	681	8	1	314	290	12	-6	761	782
3	-10	192	188	5	6	252	245	8	2	703	687	12	-5	493	487
3	-9	116	65	5	7	584	572	8	3	313	299	12	-4	131	85
3	-7	290	289	5	8	692	669	8	4	422	414	12	-3	133	115
3	-6	511	526	5	9	403	406	8	5	294	301	12	-1	144	140
3	-5	342	357	5	10	191	181	8	6	431	397	12	0	189	207
3	-4	167	176	5	12	131	134	8	7	335	350	12	4	148	154
3	-3	153	174	6	-13	341	331	8	8	285	271	12	5	580	569
3	-2	77	69	6	-12	386	428	9	-10	163	150	12	6	378	401
3	-1	245	250	6	-11	284	293	9	-9	86	104	13	-9	94	116
3	0	672	704	6	-10	135	162	9	-7	209	215	13	-8	253	235
3	1	285	228	6	-9	469	493	9	-6	229	245	13	-7	506	516
3	2	209	197	6	-8	178	159	9	-5	729	712	13	-6	300	291
3	3	106	103	6	-7	240	218	9	-4	518	530	13	-4	105	135
3	4	375	356	6	-5	315	278	9	-1	315	344	13	-3	138	159
3	5	113	86	6	-4	169	197	9	0	1057	1072	13	-1	126	138
3	6	292	293	6	-3	194	141	9	1	1003	1003	13	0	125	152
3	7	431	443	6	-2	351	340	9	2	187	173	13	2	194	176
3	8	572	557	6	-1	516	467	9	5	477	463	13	3	204	216
3	9	136	151	6	0	356	368	9	6	183	175	13	4	212	197

Table 41: Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 5****															
13	5	111	108	1	7	144	134	4	-1	90	70	7	-6	223	192
13	6	240	226	1	8	286	273	4	0	385	364	7	-5	147	91
14	-8	108	118	1	9	235	239	4	1	215	177	7	-4	704	685
14	-6	176	184	1	10	129	146	4	2	548	535	7	-3	521	513
14	-5	213	190	2	-12	71	61	4	3	838	848	7	-2	637	604
14	-2	103	78	2	-11	153	184	4	4	100	79	7	-1	282	297
14	0	327	300	2	-10	263	290	4	6	534	556	7	0	642	660
14	1	291	316	2	-9	571	593	4	7	952	926	7	1	1366	1398
14	2	174	187	2	-8	309	300	4	8	773	761	7	2	1087	1106
14	3	112	123	2	-7	413	403	4	9	207	194	7	3	303	298
14	4	221	195	2	-6	123	105	4	11	155	154	7	5	278	295
14	5	489	485	2	-5	723	718	4	12	236	235	7	6	627	635
15	-2	206	195	2	-4	1217	1206	5	-13	117	122	7	7	534	532
15	-1	431	414	2	-3	958	928	5	-11	349	349	7	8	88	88
15	0	327	326	2	-2	718	701	5	-10	672	665	7	10	105	110
15	3	193	221	2	-1	185	212	5	-9	388	388	8	-12	99	102
16	-3	90	99	2	0	241	237	5	-6	208	233	8	-9	116	136
16	-2	139	139	2	1	433	459	5	-5	196	204	8	-8	106	106
16	0	293	298	2	2	432	434	5	-4	544	511	8	-6	596	558
**H = 6****															
0	-12	86	90	2	3	343	310	5	-2	101	87	8	-5	831	820
0	-9	185	209	2	6	276	267	5	-1	272	254	8	-4	612	613
0	-8	294	299	2	7	591	566	5	0	1067	1094	8	-1	498	462
0	-7	200	168	2	8	348	334	5	1	1433	1491	8	0	1230	1188
0	-6	190	178	2	11	256	231	5	2	852	887	8	1	758	774
0	-5	1172	1134	2	12	543	565	5	3	314	333	8	3	130	103
0	-4	1584	1566	3	-11	556	549	5	4	601	581	8	4	128	127
0	-3	1141	1127	3	-10	877	886	5	5	627	613	8	5	429	409
0	-2	415	401	3	-9	409	408	5	6	999	976	8	6	200	216
0	-1	324	311	3	-6	472	484	5	7	730	732	8	9	125	119
0	0	1384	1411	3	-5	1250	1241	5	9	144	180	8	10	108	126
0	1	1717	1741	3	-4	863	841	5	10	206	220	9	-11	106	123
0	2	1215	1198	3	-3	526	496	5	11	94	115	9	-10	152	152
0	3	91	105	3	-2	180	163	6	-12	413	419	9	-9	173	184
0	4	301	331	3	-1	436	429	6	-11	478	464	9	-7	351	344
0	5	315	278	3	0	114	15	6	-10	258	240	9	-6	567	522
0	6	233	250	3	1	177	196	6	-9	178	166	9	-4	381	365
0	7	242	223	3	2	231	207	6	-8	135	119	9	-3	460	440
0	9	96	85	3	3	235	222	6	-5	398	392	9	-2	187	173
0	10	356	324	3	4	242	233	6	-3	263	266	9	-1	253	226
0	11	399	394	3	5	409	404	6	-2	485	462	9	1	106	101
0	12	265	265	3	6	289	289	6	-1	323	348	9	2	295	289
1	-11	180	172	3	8	539	508	6	0	815	840	9	3	219	171
1	-10	431	457	3	9	303	305	6	1	185	173	9	4	147	113
1	-9	145	123	3	10	114	119	6	2	545	537	9	6	259	231
1	-7	158	162	3	11	291	297	6	3	395	391	9	7	163	155
1	-6	606	594	3	12	146	148	6	4	301	320	9	8	201	218
1	-5	1058	1030	4	-13	123	123	6	5	510	505	10	-11	292	297
1	-4	404	413	4	-12	275	294	6	6	113	99	10	-10	558	583
1	-3	226	228	4	-11	491	476	6	7	430	426	10	-9	211	201
1	-2	422	466	4	-10	182	201	6	8	357	339	10	-7	255	284
1	-1	404	428	4	-9	221	204	6	9	124	106	10	-6	505	493
1	0	381	425	4	-8	292	276	7	-12	139	147	10	-5	696	659
1	1	388	373	4	-7	175	201	7	-11	110	92	10	-4	476	478
1	2	482	474	4	-6	356	346	7	-10	188	166	10	-2	301	283
1	3	438	447	4	-4	411	398	7	-9	135	125	10	-1	309	285
				4	-3	274	278	7	-8	144	93	10	0	121	153
				4	-2	139	148	7	-7	139	154	10	4	204	211



Table 41. Continued

K	L	FOBS	FCAL*	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H =		6****		**H =		7****									
10	5	409	400	0	-12	100	99	2	7	391	408	5	10	102	86
10	6	379	369	0	-11	162	152	2	8	911	872	6	-12	109	99
10	7	251	244	0	-10	133	113	2	9	395	415	6	-10	159	173
10	8	93	97	0	-9	312	301	2	11	112	92	6	-8	91	112
10	9	193	195	0	-8	537	505	2	12	142	139	6	-6	151	140
11	-10	203	208	0	-7	465	472	3	-10	443	430	6	-5	779	766
11	-8	123	114	0	-6	494	487	3	-9	641	654	6	-4	1083	1081
11	-7	471	454	0	-4	933	933	3	-8	341	322	6	-3	559	543
11	-6	506	479	0	-3	1470	1468	3	-6	167	154	6	-1	417	398
11	-5	400	397	0	-2	851	858	3	-4	310	279	6	0	1022	1036
11	0	242	200	0	-1	80	52	3	-3	129	136	6	1	1503	1534
11	2	270	254	0	1	503	534	3	-2	242	218	6	2	662	689
11	3	219	225	0	2	1114	1133	3	-1	356	309	6	3	191	154
11	4	276	256	0	3	400	416	3	0	301	306	6	4	208	229
11	5	203	230	0	4	108	63	3	1	637	631	6	5	525	500
11	7	318	339	0	6	440	433	3	2	805	806	6	6	312	300
11	8	377	397	0	7	283	304	3	3	216	228	6	7	215	205
12	-9	165	188	0	8	543	511	3	5	278	268	6	10	111	113
12	-8	200	194	0	9	390	381	3	6	598	591	7	-11	84	58
12	-6	143	123	0	11	212	211	3	7	910	875	7	-10	236	244
12	-5	167	184	0	12	290	308	3	8	691	688	7	-9	91	97
12	-4	201	174	1	-11	109	112	3	9	129	103	7	-7	315	319
12	-3	108	83	1	-10	640	637	3	10	123	69	7	-6	670	650
12	0	104	106	1	-9	738	737	4	-12	134	120	7	-5	751	733
12	1	358	401	1	-8	351	369	4	-11	473	484	7	-3	475	495
12	2	412	380	1	-7	277	233	4	-10	690	692	7	-2	267	247
12	5	348	364	1	-6	171	133	4	-9	226	215	7	-1	264	240
12	6	577	570	1	-5	1055	1027	4	-8	143	152	7	0	873	882
12	7	479	479	1	-4	1161	1191	4	-7	111	98	7	2	631	654
13	-8	91	65	1	-3	733	761	4	-4	197	180	7	4	229	206
13	-7	78	81	1	-2	233	240	4	-2	142	172	7	5	107	97
13	-6	173	157	1	-1	183	191	4	-1	437	416	7	7	86	25
13	-4	120	86	1	1	488	502	4	0	868	878	7	8	180	175
13	-3	131	140	1	2	317	319	4	1	458	476	7	9	188	203
13	-1	330	311	1	5	114	115	4	3	774	774	7	10	152	145
13	0	514	527	1	6	359	362	4	4	509	501	8	-10	154	159
13	1	357	342	1	7	628	604	4	5	353	407	8	-9	285	301
13	2	129	111	1	8	146	136	4	6	271	285	8	-8	178	181
13	3	152	144	1	9	165	146	4	8	246	230	8	-7	215	218
13	4	349	330	1	10	315	305	4	9	104	86	8	-5	546	570
13	5	543	581	1	11	255	273	4	11	75	75	8	-4	877	850
13	6	352	370	1	12	352	350	5	-12	146	144	8	-3	679	680
14	-6	85	53	2	-12	92	105	5	-9	183	199	8	0	441	442
14	-3	101	118	2	-11	461	478	5	-7	257	268	8	1	797	748
14	-2	180	193	2	-10	619	624	5	-4	432	419	8	2	275	276
14	-1	296	311	2	-8	133	141	5	-3	797	780	8	3	201	220
14	1	270	268	2	-6	483	476	5	-2	513	519	8	4	112	98
14	2	156	159	2	-5	862	843	5	0	162	186	8	6	314	316
14	3	193	197	2	-4	201	214	5	1	609	608	8	7	293	286
14	4	174	183	2	-2	230	222	5	2	1241	1242	8	8	135	130
15	-5	310	272	2	-1	223	231	5	3	478	449	9	-11	408	400
15	-4	180	191	2	0	185	176	5	4	164	191	9	-10	581	588
15	-1	281	278	2	1	81	84	5	5	184	199	9	-9	196	194
15	0	571	604	2	2	422	417	5	6	522	502	9	-7	255	241
15	1	341	349	2	3	173	201	5	7	507	500	9	-6	665	660
15	2	81	79	2	4	318	326	5	8	227	229	9	-5	766	756
												9	-4	559	534



Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	7****		13	5	256	286	2	-5	479	461	5	1	425	416
9	0	206	216	14	-6	382	397	2	-4	353	335	5	2	177	183
9	1	391	359	14	-5	433	429	2	-3	175	143	5	3	323	325
9	5	396	398	14	-4	178	156	2	0	139	135	5	8	124	132
9	6	186	192	14	-1	416	422	2	1	504	533	5	9	203	194
9	7	117	142	14	0	573	584	2	2	303	297	5	10	138	133
9	8	232	221	14	1	265	282	2	3	150	107	6	-11	135	133
9	9	115	116	14	3	108	94	2	4	215	199	6	-9	192	182
10	-10	116	118	15	-3	123	146	2	5	237	234	6	-8	316	316
10	-9	177	167	15	-2	176	168	2	6	327	352	6	-7	440	456
10	-7	95	116	15	-1	160	138	2	7	532	527	6	-6	337	335
10	-6	115	92	15	0	142	144	2	8	236	224	6	-5	176	163
10	-5	136	109		**H =	8****		2	9	267	258	6	-4	951	925
10	-4	139	140	0	-11	338	343	2	10	221	203	6	-3	1083	1074
10	-2	115	132	0	-10	652	683	2	11	101	82	6	-2	336	335
10	1	468	422	0	-9	508	490	3	-12	78	84	6	0	253	207
10	2	393	392	0	-8	125	133	3	-11	327	334	6	1	756	757
10	5	248	244	0	-7	171	189	3	-10	341	336	6	2	1031	1040
10	6	480	492	0	-6	237	219	3	-9	144	153	6	3	111	58
10	7	564	558	0	-5	706	690	3	-7	171	139	6	5	106	78
10	8	275	283	0	-4	476	468	3	-6	140	139	6	7	190	185
11	-10	439	491	0	-2	428	453	3	-4	225	200	6	8	355	348
11	-9	88	91	0	-1	171	146	3	-3	316	320	6	9	236	218
11	-8	157	158	0	2	261	221	3	-2	450	431	7	-11	201	182
11	-7	153	173	0	3	398	395	3	-1	247	230	7	-10	561	569
11	-6	251	257	0	4	177	169	3	1	244	244	7	-9	436	409
11	-2	121	102	0	5	354	377	3	2	695	727	7	-8	226	238
11	-1	239	205	0	6	403	399	3	3	804	774	7	-6	316	307
11	0	449	480	0	8	430	408	3	4	453	449	7	-5	896	863
11	1	575	563	0	9	521	524	3	5	180	174	7	-4	1074	1016
11	3	185	193	0	10	391	376	3	7	440	426	7	-3	567	568
11	4	247	236	0	11	84	87	3	8	450	445	7	-1	117	173
11	5	458	501	1	-12	213	201	3	9	270	259	7	0	377	388
11	6	496	496	1	-11	299	312	3	11	101	87	7	1	534	517
11	7	243	244	1	-9	572	567	4	-10	152	177	7	3	287	265
12	-9	79	65	1	-8	720	686	4	-5	569	570	7	5	139	140
12	-8	90	101	1	-7	356	358	4	-4	681	675	7	6	208	230
12	-6	167	161	1	-6	374	381	4	-3	628	630	7	7	329	320
12	-5	172	145	1	-4	621	640	4	-2	165	162	7	9	214	228
12	-2	218	216	1	-3	388	423	4	-1	375	352	8	-11	431	447
12	-1	499	496	1	-2	214	227	4	0	718	720	8	-10	292	288
12	0	280	288	1	-1	82	92	4	1	1066	1108	8	-8	156	164
12	1	106	51	1	0	207	188	4	2	916	931	8	-7	279	271
12	2	398	391	1	1	179	165	4	3	300	322	8	-6	365	372
12	3	335	308	1	2	457	453	4	5	96	90	8	-5	226	227
12	4	179	187	1	3	611	634	4	6	368	357	8	-3	460	446
12	5	90	111	1	4	604	595	4	7	338	321	8	-2	280	247
12	6	86	93	1	6	298	309	4	8	278	265	8	-1	182	137
13	-7	126	120	1	7	811	810	5	-10	146	161	8	0	201	200
13	-5	191	200	1	8	926	888	5	-9	157	124	8	1	140	119
13	-4	202	164	1	9	364	365	5	-7	252	260	8	2	198	179
13	-3	148	132	1	11	97	108	5	-6	455	444	8	5	143	171
13	-2	231	243	2	-11	138	134	5	-5	736	722	8	6	113	77
13	0	556	539	2	-10	582	564	5	-4	502	489	8	7	440	452
13	1	653	640	2	-9	775	761	5	-2	364	375	8	8	502	508
13	2	452	459	2	-8	353	342	5	-1	631	637	8	9	172	178
13	3	95	109	2	-7	106	99	5	0	525	515	9	-10	403	390

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
9	-9	381	393	13	3	173	196	2	2	1055	1063	6	-3	449	425
9	-8	248	250	14	-5	413	411	2	3	892	906	6	-2	359	334
9	-7	118	85	14	-4	406	420	2	4	384	377	6	-1	201	191
9	-5	278	262	14	-3	131	116	2	5	95	101	6	0	147	148
9	-4	227	211	14	-2	105	118	2	6	178	151	6	1	98	93
9	-3	193	190	14	-1	98	104	2	7	471	469	6	2	135	140
9	-2	186	140	14	0	309	365	2	8	544	535	6	4	298	296
9	0	160	196	14	1	27	339	2	9	225	238	6	5	312	305
9	1	599	555	14	2	1	133	2	10	101	94	6	6	178	174
9	2	425	44	14	3	9****		3	-5	566	533	6	7	102	97
9	4	163	17	0	0	381	395	3	-4	571	557	6	8	449	437
9	5	365	34	0	0	723	744	3	-3	217	226	6	9	442	433
9	6	516	514	0	0	617	605	3	-2	197	181	7	-10	139	151
9	7	604	636	0	7	202	200	3	-1	192	199	7	-9	438	437
9	8	118	123	0	-5	364	366	3	0	438	419	7	-8	446	436
10	-10	248	259	0	-4	436	420	3	1	826	831	7	-7	349	321
10	-2	335	316	0	-3	535	497	3	2	448	421	7	-6	157	174
10	-1	165	204	0	-1	218	200	4	-10	78	80	7	-5	93	18
10	0	396	388	0	0	97	107	4	-9	98	100	7	-4	538	573
10	1	216	163	0	1	342	351	4	-8	334	351	7	-3	630	623
10	2	227	249	0	2	675	708	4	-7	197	174	7	0	261	235
10	3	260	252	0	3	445	424	4	-6	283	286	7	2	260	241
10	4	210	184	0	5	177	163	4	-5	194	206	7	3	241	251
10	5	164	171	0	6	408	398	4	-4	313	298	7	4	208	201
10	6	186	199	0	7	661	625	4	-3	722	718	7	6	310	323
10	7	186	206	0	8	290	278	4	-2	641	650	7	7	634	615
11	-9	99	91	0	9	181	173	4	-1	244	252	7	8	547	559
11	-6	97	82	0	10	266	265	4	0	208	232	8	-10	508	514
11	-4	213	198	1	-11	295	297	4	1	170	191	8	-9	374	369
11	-3	278	318	1	-10	556	559	4	2	758	728	8	-8	104	99
11	-2	136	122	1	-9	352	368	4	3	469	445	8	-6	234	218
11	0	266	270	1	-8	133	163	4	4	130	118	8	-5	378	363
11	1	503	505	1	-7	105	73	4	8	171	157	8	-4	115	130
11	2	548	566	1	-6	114	97	4	9	173	161	8	-1	101	63
11	3	368	348	1	-3	113	164	4	10	71	56	8	0	172	155
11	5	115	113	1	-2	178	180	5	-10	330	341	8	1	591	585
11	6	321	318	1	-1	197	184	5	-9	512	508	8	2	322	337
12	-6	221	224	1	0	339	328	5	-8	294	299	8	4	194	219
12	-5	443	446	1	1	620	622	5	-6	164	137	8	5	190	220
12	-4	429	449	1	2	249	255	5	-5	746	744	8	6	390	373
12	-1	329	336	1	3	738	756	5	-4	1093	1091	8	7	291	301
12	0	629	636	1	4	564	542	5	-3	755	747	8	8	160	154
12	1	457	470	1	5	258	269	5	-1	122	153	9	-8	84	66
12	2	160	139	1	6	135	130	5	1	496	518	9	-6	93	55
12	4	160	180	1	8	400	394	5	2	212	211	9	-5	127	85
12	5	205	203	1	9	596	568	5	5	219	234	9	-3	340	305
13	-7	108	123	1	10	211	210	5	6	235	214	9	-2	185	161
13	-6	404	404	2	-11	187	176	5	7	265	279	9	-1	159	94
13	-5	312	367	2	-9	282	296	5	8	125	132	9	1	339	303
13	-4	97	118	2	-8	205	216	6	-11	396	420	9	2	729	759
13	-3	245	256	2	-5	186	168	6	-10	626	655	9	3	269	248
13	-2	194	195	2	-4	266	279	6	-9	250	260	9	7	315	334
13	-1	420	440	2	-3	432	443	6	-8	174	174	10	-8	97	85
13	0	221	214	2	-2	326	348	6	-7	278	283	10	-6	152	158
13	1	131	142	2	-1	86	82	6	-6	385	389	10	-5	322	321
13	2	302	315	2	0	126	48	6	-5	585	568	10	-4	427	426
				2	1	486	501	6	-4	348	351	10	-3	280	242

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 9****															
10	-1	171	145	1	-4	392	386	5	-10	194	184	9	-7	108	90
10	0	445	463	1	-3	591	582	5	-9	251	248	9	-6	171	186
10	1	735	738	1	-2	416	408	5	-8	532	532	9	-5	190	178
10	2	361	339	1	-1	192	216	5	-7	337	328	9	-4	239	248
10	4	133	132	1	0	247	223	5	-6	200	182	9	-2	210	156
10	5	88	108	1	1	535	543	5	-5	183	174	9	-1	234	228
10	6	173	172	1	2	805	811	5	-4	274	265	9	0	311	315
11	-8	90	64	1	3	515	505	5	-3	483	503	9	1	449	466
11	-7	183	168	1	5	197	172	5	-2	243	252	9	2	228	203
11	-6	311	318	1	6	246	228	5	0	155	135	9	3	102	94
11	-5	365	350	1	7	213	223	5	2	196	180	9	4	117	113
11	-3	281	280	1	8	215	222	5	3	224	229	9	5	133	126
11	-2	254	283	1	9	133	123	5	4	384	383	9	6	136	145
11	-1	379	338	2	-10	106	111	5	6	165	163	10	-8	129	138
11	0	400	397	2	-8	158	166	5	7	460	462	10	-7	193	198
11	2	194	222	2	-7	176	175	5	8	702	690	10	-6	157	152
11	3	283	278	2	-5	227	218	6	-10	518	524	10	-4	303	308
12	-7	146	138	2	-4	262	256	6	-9	607	603	10	-3	406	414
12	-6	182	183	2	-3	224	251	6	-8	381	366	10	-2	276	305
12	-5	127	120	2	-2	331	331	6	-6	276	277	10	-1	150	171
12	-4	498	491	2	-1	255	235	6	-5	264	243	10	2	340	374
12	-3	367	368	2	0	268	271	6	-4	529	499	10	3	169	193
12	-2	150	136	2	1	352	360	6	-3	394	373	11	-7	101	98
12	-1	112	92	2	2	136	125	6	-2	288	243	11	-6	203	217
12	0	196	193	2	3	488	496	6	0	121	124	11	-5	467	491
12	1	436	446	2	4	371	355	6	1	335	343	11	-4	557	562
12	2	330	333	2	5	255	248	6	2	326	317	11	-3	159	152
13	-5	613	603	2	8	128	123	6	3	243	218	11	0	283	282
13	-4	407	419	2	9	158	143	6	5	171	164	11	1	281	261
13	-2	98	85	3	-10	149	133	6	6	325	327	11	2	86	70
13	-1	248	256	3	-9	239	243	6	7	351	351	12	-5	404	426
13	0	326	340	3	-8	414	396	6	8	115	116	12	-3	190	214
13	1	223	182	3	-7	147	135	7	-9	181	194	12	-2	190	182
**H = 10****				3	-5	322	306	7	-8	121	117	12	-1	100	134
0	-10	163	170	3	-4	773	763	7	-7	215	235	**H = 11****			
0	-9	195	211	3	-3	991	961	7	-6	166	138	0	-9	84	107
0	-8	457	457	3	-2	460	459	7	-5	119	133	0	-6	376	364
0	-7	140	115	3	-1	196	203	7	-4	96	49	0	-5	395	383
0	-6	122	105	3	0	109	139	7	-4	96	49	0	-4	296	277
0	-5	118	112	3	0	109	139	7	-1	132	163	0	-4	296	277
0	-4	145	170	3	1	286	302	7	0	272	273	0	-3	408	409
0	-3	293	293	3	1	286	302	7	0	272	273	0	-3	408	409
0	-2	514	544	3	2	473	480	7	1	173	169	0	-2	276	257
0	-1	361	365	3	2	473	480	7	1	173	169	0	-2	276	257
0	0	262	306	3	3	326	348	7	2	187	141	0	-1	448	460
0	2	513	524	3	3	326	348	7	2	187	141	0	-1	448	460
0	3	1017	1011	3	6	209	208	7	3	537	499	0	0	343	377
0	4	608	617	4	-10	397	375	7	4	547	532	0	1	230	221
0	6	118	119	4	-9	435	456	7	5	182	202	0	1	230	221
0	7	392	387	4	-7	154	147	7	6	114	104	0	3	376	383
0	8	623	585	4	-6	293	309	7	7	250	241	0	4	568	574
0	9	433	415	4	-5	608	599	8	-9	226	249	0	5	400	386
1	-10	123	104	4	-4	605	594	8	-8	202	222	0	8	74	60
1	-9	338	315	4	-3	134	130	8	-8	202	222	0	9	165	168
1	-7	123	116	4	-2	226	238	8	-4	135	125	1	-8	180	178
1	-6	116	119	4	-1	110	81	8	-3	463	446	1	-7	276	294
				4	1	216	175	8	-2	271	279	1	-6	92	77
				4	4	126	140	8	1	424	429	1	-4	105	75
				4	5	160	182	8	2	642	689	1	-3	703	676
				4	8	174	163	8	3	551	519	1	-2	902	912
				4	9	327	318	8	6	251	242	1	-1	343	339
								8	7	428	439	1	2	539	525

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 11****				6	-1	243	256	0	-1	118	108	5	5	245	242
1	3	653	659	6	0	273	245	0	0	169	181	5	6	154	163
1	4	335	350	6	1	154	178	0	1	257	231	6	-5	245	251
1	5	146	133	6	2	483	525	0	2	466	481	6	-4	342	342
1	6	98	89	6	3	599	608	0	3	260	273	6	-2	231	222
2	-9	301	315	6	4	246	284	0	5	101	74	6	-1	187	216
2	-8	304	299	6	6	117	118	0	7	89	75	6	0	300	317
2	-7	214	177	6	7	473	474	1	-8	122	114	6	1	163	176
2	-5	144	148	7	-8	113	119	1	-6	277	267	6	3	444	432
2	-4	722	720	7	-5	93	97	1	-5	305	312	6	4	412	428
2	-3	866	867	7	-4	321	340	1	-4	387	357	6	5	91	105
2	-2	252	256	7	-3	349	326	1	-3	281	262	7	-7	181	186
2	-1	146	144	7	-1	139	124	1	-2	213	200	7	-6	97	71
2	1	353	371	7	0	372	335	1	-1	298	281	7	-4	248	234
2	2	384	389	7	1	615	597	1	0	228	216	7	-3	600	574
2	3	182	161	7	2	485	485	1	1	210	199	7	-2	435	432
2	5	107	120	7	3	120	115	1	2	129	121	7	-1	229	217
3	-8	313	307	7	4	273	273	1	3	176	160	7	1	320	307
3	-7	312	305	7	5	189	178	2	-8	484	479	7	2	540	539
3	-6	165	159	7	6	224	249	2	-7	426	439	7	3	529	547
3	-5	229	223	8	-7	125	113	2	-6	111	86	7	4	144	141
3	-4	291	275	8	-6	181	176	2	-4	249	229	8	-5	313	299
3	-3	142	127	8	-5	149	154	2	-3	395	387	8	-4	479	491
3	-2	440	409	8	-3	135	165	2	-2	386	401	8	-3	446	468
3	0	128	89	8	-2	242	229	2	-1	111	103	8	-1	104	126
3	3	137	112	8	-1	119	124	2	2	107	106	8	0	204	233
3	7	230	232	8	0	290	306	2	5	115	105	8	1	306	293
3	8	352	335	8	2	128	127	2	6	112	113	8	2	271	300
4	-9	519	536	8	3	408	408	2	7	209	205	9	-5	190	169
4	-8	499	482	8	4	176	208	3	-8	405	397	9	-3	222	224
4	-7	108	101	8	6	91	99	3	-5	102	64	9	-2	107	90
4	-4	314	310	9	-5	276	260	3	-4	291	272	9	2	84	41
4	-3	526	546	9	-4	567	565	3	-3	334	328	10	-3	235	253
4	0	149	158	9	-3	513	546	3	0	133	139	10	0	82	63
4	1	223	232	9	-2	142	173	3	4	233	241	**H = 13****			
4	2	171	164	9	0	205	173	3	5	243	250	0	-7	323	305
4	5	118	127	9	1	274	267	3	6	146	161	0	-6	254	256
4	6	268	260	9	2	427	427	3	7	211	215	0	-5	135	140
4	7	305	299	9	3	105	153	4	-8	169	162	0	-3	381	381
4	8	344	345	10	-6	194	216	4	-7	153	174	0	-2	660	643
5	-9	391	410	10	-5	481	493	4	-4	112	87	0	-1	358	378
5	-7	220	210	10	-4	329	278	4	-2	180	180	0	2	128	118
5	-6	171	167	10	-3	85	62	4	0	100	105	0	5	91	85
5	-4	195	166	10	0	138	162	4	2	311	293	1	-7	408	410
5	-2	130	125	10	1	188	156	4	3	521	536	1	-5	95	106
5	-1	211	221	11	-4	276	283	4	4	353	368	1	-4	269	246
5	0	233	227	11	-3	261	243	4	5	80	79	1	-3	615	580
5	1	380	382	11	-1	84	46	4	6	124	111	1	-2	284	247
5	3	366	343	11	2	111	131	5	-8	224	206	1	-1	88	77
5	4	480	450	**H = 12****				5	-6	153	146	1	0	97	98
5	5	335	347	0	-8	356	361	5	-4	252	265	1	5	96	85
5	6	148	151	0	-7	284	295	5	-3	264	245	1	6	110	106
6	-9	198	203	0	-6	116	102	5	-2	206	203	2	-7	106	97
6	-8	242	221	0	-5	228	210	5	0	148	142	2	-4	280	285
6	-7	182	180	0	-4	330	336	5	1	519	518	2	-3	118	111
6	-3	102	86	0	-3	614	608	5	2	570	576	2	2	110	125
6	-2	238	263	0	-2	490	473	5	3	388	361	2	3	231	213

Table 41. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 13****															
2	4	331	330	4	4	302	303	7	-4	253	256	2	3	222	231
2	5	238	237	4	5	224	221	7	-2	248	265	3	-4	85	95
3	-7	203	191	5	-6	102	99	7	-1	223	223	3	-3	96	108
3	-5	79	78	5	-5	101	89	7	0	118	113	3	-2	254	259
3	-2	105	122	5	-3	385	382	7	3	147	157	3	-1	280	296
3	-1	97	93	5	-2	534	555	8	-3	445	455	3	0	185	202
3	0	118	139	5	-1	228	212	8	-2	263	273	3	2	101	77
3	1	201	198	5	1	97	94	**H = 14****				3	3	286	283
3	2	330	328	5	2	395	396	0	-4	118	133	4	-4	233	222
3	3	440	447	5	3	593	586	0	-3	90	108	4	-3	504	469
3	4	265	260	5	4	363	351	0	-1	77	67	4	-2	383	371
4	-5	189	193	6	-5	134	118	0	0	110	93	4	-1	146	150
4	-4	176	172	6	-4	423	420	0	1	95	90	4	0	208	203
4	-3	235	246	6	-3	646	657	1	-3	118	123	4	1	130	133
4	-2	154	145	6	-2	210	207	1	-2	168	156	4	2	302	301
4	-1	254	251	6	0	195	189	1	2	146	145	5	-3	214	230
4	0	243	222	6	1	286	294	1	3	343	343	5	-2	81	67
4	1	212	219	6	2	435	453	2	0	147	131	5	-1	331	336
4	2	206	211	6	3	314	336	2	1	178	181	5	0	145	151
4	3	122	102	7	-5	266	268	2	2	217	201	6	-1	282	300

Table 42. 10\*(Fobs vs. Fcal) For Trans-[RhCl(CO)(DPM)]2.

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -10****				-8	-2	29	37	-7	-2	326	329	-11	-2	202	197
-9	-1	65	75	-8	-1	416	421	-7	-1	572	569	-11	-1	204	191
-8	-1	27	23	-7	-4	49	67	-6	-4	317	324	-10	-4	95	83
-7	-1	111	124	-7	-3	203	197	-6	-3	75	52	-10	-3	67	59
-6	-2	172	152	-7	-1	85	98	-6	-2	39	39	-10	-2	134	135
-6	-1	140	140	-6	-4	87	79	-6	-1	188	182	-10	-1	208	211
-5	-2	231	223	-6	-3	268	276	-5	-5	25	17	-9	-5	185	193
-5	-1	83	88	-6	-2	107	108	-5	-4	172	177	-9	-4	193	195
-4	-2	211	219	-6	-1	181	190	-5	-3	184	185	-9	-3	26	2
-4	-1	63	56	-5	-4	226	210	-5	-2	54	36	-9	-2	358	352
-3	-1	74	75	-5	-3	350	368	-5	-1	126	108	-9	-1	357	347
-2	-1	79	94	-5	-2	177	176	-4	-5	28	11	-8	-5	273	288
-1	-1	114	110	-5	-1	369	368	-4	-4	145	142	-8	-4	532	525
**H = -9****				-4	-4	271	275	-4	-3	317	294	-8	-3	61	63
-11	-1	238	258	-4	-3	461	457	-4	-2	76	67	-8	-2	278	295
-10	-1	174	173	-4	-2	255	258	-4	-1	168	163	-8	-1	417	416
-9	-2	33	23	-4	-1	356	379	-3	-4	280	276	-7	-6	27	13
-9	-1	144	160	-3	-4	199	207	-3	-3	372	380	-7	-5	325	306
-8	-2	84	75	-3	-3	540	556	-3	-2	428	451	-7	-4	383	398
-8	-1	80	78	-3	-2	166	165	-3	-1	169	155	-7	-3	208	204
-7	-3	137	143	-3	-1	79	84	-2	-5	206	211	-7	-2	568	565
-7	-2	97	85	-2	-4	81	82	-2	-4	159	146	-7	-1	806	829
-7	-1	28	31	-2	-3	235	234	-2	-3	336	326	-6	-6	167	165
-6	-3	280	287	-2	-2	135	110	-2	-2	380	373	-6	-5	252	260
-6	-2	143	139	-1	-4	26	6	-2	-1	130	118	-6	-4	432	430
-6	-1	213	218	-1	-2	151	143	-1	-5	190	177	-6	-3	385	398
-5	-3	332	336	0	-4	57	63	-1	-4	52	36	-6	-2	263	272
-5	-2	144	135	0	-2	95	92	-1	-3	243	230	-6	-1	388	384
-5	-1	300	310 <sup>7</sup>	0	-1	307	311	-1	-2	209	237	-5	-6	136	146
-4	-3	386	403	1	-2	116	109	-1	-1	269	261	-5	-5	106	108
-4	-2	252	250	1	-1	326	319	0	-5	131	128	-5	-4	270	253
-4	-1	179	161	2	-3	76	78	0	-4	163	182	-5	-3	40	38
-3	-3	231	231	2	-2	305	293	0	-3	34	29	-5	-1	152	143
-3	-2	199	180	2	-1	514	535	0	-2	311	312	-4	-6	115	113
-3	-1	44	41	3	-2	260	258	0	-1	221	220	-4	-5	51	55
-2	-3	88	81	3	-1	440	442	1	-4	169	171	-4	-4	111	115
-2	-2	160	165	4	-1	324	321	1	-3	86	78	-4	-3	30	33
-2	-1	98	91	**H = -7****				1	-2	290	294	-4	-2	55	49
-1	-3	76	80	-12	-2	34	38	1	-1	82	85	-4	-1	46	42
-1	-2	143	143	-12	-1	123	125	2	-4	181	190	-3	-6	118	109
-1	-1	204	200	-11	-3	60	67	2	-2	182	176	-3	-4	38	36
0	-2	227	220	-11	-2	51	35	2	-1	431	413	-3	-3	326	328
0	-1	165	181	-11	-1	144	137	3	-4	300	310	-3	-2	127	123
1	-2	288	295	-10	-3	82	66	3	-3	34	29	-3	-1	28	31
1	-1	288	289	-10	-2	180	199	3	-2	376	383	-2	-6	186	193
2	-1	371	378	-10	-1	303	288	3	-1	577	565	-2	-5	131	136
**H = -8****				-9	-4	331	358	4	-3	97	93	-2	-4	64	68
-12	-1	91	91	-9	-3	98	83	4	-2	313	316	-2	-3	499	508
-11	-2	203	204	-9	-2	282	279	4	-1	324	321	-2	-2	438	433
-11	-1	229	233	-9	-1	423	442	5	-2	129	132	-2	-1	100	102
-10	-2	277	268	-8	-4	326	320	5	-1	241	244	-1	-6	340	349
-10	-1	407	421	-8	-3	187	177	6	-1	123	121	-1	-5	325	329
-9	-3	40	34	-8	-2	231	256	**H = -6****				-1	-4	56	61
-9	-2	75	76	-8	-1	680	688	-13	-1	77	76	-1	-3	363	353
-9	-1	322	330	-7	-5	132	142	-12	-2	255	263	-1	-2	751	756
-8	-4	138	125	-7	-4	289	310	-12	-1	221	206	-1	-1	181	187
-8	-3	150	143	-7	-3	225	222	-11	-3	55	54	0	-6	248	239

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H =	-6****			-7	-4	261	273	2	-6	174	160	-7	-7	167	183
0	-5	313	304	-7	-3	66	73	2	-5	337	340	-7	-6	110	127
0	-4	158	158	-7	-2	328	323	2	-4	286	278	-7	-5	244	232
0	-3	302	289	-7	-1	419	405	2	-3	140	135	-7	-4	206	201
0	-2	504	489	-6	-7	303	283	2	-2	251	244	-7	-3	56	59
0	-1	381	376	-6	-6	41	44	2	-1	50	67	-7	-2	138	127
1	-6	41	47	-6	-5	236	246	3	-5	190	193	-7	-1	280	273
1	-5	303	302	-6	-4	558	572	3	-4	116	114	-6	-7	218	214
1	-4	216	202	-6	-3	252	236	3	-3	144	160	-6	-5	247	238
1	-3	202	200	-6	-2	240	237	3	-2	34	35	-6	-4	72	73
1	-2	409	425	-6	-1	512	532	3	-1	75	83	-6	-3	101	98
1	-1	320	330	-5	-7	314	319	4	-5	116	129	-6	-2	273	273
2	-5	172	179	-5	-6	128	146	4	-4	142	128	-6	-1	515	525
2	-4	206	203	-5	-5	196	206	4	-3	34	28	-5	-7	206	193
2	-2	97	91	-5	-4	494	476	4	-2	221	219	-5	-6	79	79
2	-1	110	124	-5	-3	322	329	4	-1	278	265	-5	-5	226	222
3	-5	141	138	-5	-2	104	98	5	-5	201	221	-5	-4	763	772
3	-4	114	104	-5	-1	459	452	5	-4	321	327	-5	-3	421	444
3	-3	129	134	-4	-7	197	204	5	-2	270	271	-5	-2	177	170
3	-2	282	280	-4	-6	218	208	5	-1	392	402	-5	-1	662	655
3	-1	360	377	-4	-5	104	108	6	-4	325	325	-4	-8	219	221
4	-4	224	233	-4	-4	44	37	6	-3	168	167	-4	-7	217	226
4	-2	331	334	-4	-3	276	268	6	-2	150	143	-4	-6	216	207
4	-1	379	361	-4	-2	247	249	6	-1	499	494	-4	-5	49	32
5	-4	303	316	-4	-1	153	155	7	-3	228	224	-4	-4	527	534
5	-3	97	101	-3	-7	65	66	7	-2	59	53	-4	-3	477	479
5	-2	201	200	-3	-6	164	177	7	-1	401	402	-4	-2	72	80
5	-1	401	405	-3	-5	133	136	8	-2	210	216	-4	-1	486	513
6	-3	161	173	-3	-4	28	20	8	-1	135	131	-3	-8	71	83
6	-1	287	296	-3	-3	91	71	**H =	-4****			-3	-7	144	144
7	-1	112	116	-3	-2	361	360	-13	-2	169	166	-3	-6	244	240
**H =	-5****			-3	-1	303	298	-13	-1	23	10	-3	-5	177	196
-13	-2	297	296	-2	-6	116	113	-12	-3	333	318	-3	-4	153	152
-13	-1	30	40	-2	-5	127	107	-12	-2	365	354	-3	-3	473	494
-12	-3	331	322	-2	-4	92	80	-11	-5	316	302	-3	-2	246	243
-12	-2	383	368	-2	-3	405	428	-11	-4	47	45	-3	-1	460	450
-12	-1	149	142	-2	-2	439	444	-11	-3	365	351	-2	-8	160	153
-11	-4	130	127	-2	-1	159	140	-11	-2	427	428	-2	-6	226	233
-11	-3	181	191	-1	-7	98	103	-11	-1	38	39	-2	-5	315	316
-11	-2	362	363	-1	-6	272	280	-10	-5	385	381	-2	-4	55	69
-11	-1	105	116	-1	-5	258	285	-10	-4	74	73	-2	-3	432	425
-10	-5	139	143	-1	-4	50	44	-10	-3	321	321	-2	-2	457	454
-10	-4	199	192	-1	-3	636	634	-10	-2	468	459	-2	-1	144	142
-10	-3	147	147	-1	-2	463	472	-10	-1	185	178	-1	-8	139	138
-10	-2	370	378	-1	-1	100	83	-9	-6	105	108	-1	-7	47	43
-10	-1	82	80	0	-7	79	75	-9	-5	319	299	-1	-6	294	309
-9	-5	107	100	0	-6	385	376	-9	-4	160	151	-1	-5	359	377
-9	-4	108	122	0	-5	350	328	-9	-3	197	194	-1	-4	135	142
-9	-3	162	172	0	-4	43	23	-9	-2	336	343	-1	-3	398	401
-9	-2	289	280	0	-3	578	566	-9	-1	114	114	-1	-2	156	155
-9	-1	173	170	0	-2	753	762	-8	-7	173	160	-1	-1	31	40
-8	-5	320	343	1	-6	342	327	-8	-6	93	112	0	-8	149	159
-8	-4	234	224	1	-5	339	338	-8	-5	85	86	0	-6	491	501
-8	-3	81	83	1	-4	95	108	-8	-4	142	143	0	-5	354	358
-8	-2	212	214	1	-3	411	422	-8	-3	36	34	0	-4	287	305
-8	-1	281	290	1	-2	700	697	-8	-2	210	223	0	-3	491	508
-7	-5	441	433	1	-1	181	201	-8	-1	118	114	0	-2	530	522





Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-2****													
-7	-6	154	138	-1	-2	253	253	7	-6	108	122	-7	-3	294	283
-7	-5	367	383	-1	-1	165	150	7	-5	193	196	-7	-2	770	799
-7	-4	356	359	0	-9	216	200	7	-4	255	273	-7	-1	604	603
-7	-3	36	2	0	-8	59	54	7	-2	107	103	-6	-9	49	47
-7	-2	393	400	0	-7	268	277	7	-1	47	44	-6	-8	267	270
-7	-1	696	700	0	-6	276	275	8	-6	71	74	-6	-7	185	193
-6	-8	66	69	0	-5	55	35	8	-5	162	167	-6	-6	110	111
-6	-7	65	63	0	-4	151	148	8	-4	227	225	-6	-5	603	612
-6	-6	85	91	0	-3	106	89	8	-3	30	21	-6	-4	442	484
-6	-5	184	190	0	-2	36	37	8	-2	141	155	-6	-3	107	105
-6	-4	376	394	0	-1	22	15	8	-1	193	199	-6	-2	803	795
-6	-3	120	118	1	-9	82	88	9	-5	203	207	-6	-1	742	722
-6	-2	411	388	1	-8	29	32	9	-4	307	319	-5	-8	248	272
-6	-1	434	462	1	-7	177	164	9	-3	289	278	-5	-7	414	404
-5	-8	44	43	1	-6	129	143	9	-2	36	26	-5	-6	100	108
-5	-7	253	246	1	-5	68	42	9	-1	430	421	-5	-5	300	315
-5	-6	202	224	1	-4	155	150	10	-4	237	250	-5	-4	666	675
-5	-5	33	29	1	-3	134	116	10	-3	338	336	-5	-3	110	98
-5	-4	268	264	1	-2	420	414	10	-2	44	35	-5	-2	121	133
-5	-3	168	173	1	-1	59	58	10	-1	310	320	-5	-1	79	53
-5	-2	136	151	2	-9	122	120	11	-2	210	196	-4	-9	145	153
-5	-1	363	379	2	-8	150	146	11	-1	100	101	-4	-8	105	106
-4	-9	129	113	2	-7	124	134		**H =	-1****		-4	-7	231	231
-4	-8	82	70	2	-6	170	177	-13	-1	250	267	-4	-6	59	63
-4	-7	109	112	2	-5	156	153	-12	-4	211	205	-4	-5	120	122
-4	-6	244	249	2	-4	235	215	-12	-3	260	268	-4	-4	331	341
-4	-5	186	190	2	-3	481	455	-12	-2	95	98	-4	-3	70	71
-4	-4	527	553	2	-2	408	427	-12	-1	64	53	-4	-2	59	46
-4	-3	326	338	2	-1	252	242	-11	-5	29	14	-4	-1	521	507
-4	-2	405	388	3	-8	169	173	-11	-3	99	102	-3	-9	40	27
-4	-1	1061	1077	3	-6	286	278	-11	-2	127	134	-3	-8	239	248
-3	-9	140	131	3	-5	429	413	-11	-1	117	82	-3	-7	219	231
-3	-8	130	120	3	-4	370	367	-10	-6	34	60	-3	-6	291	276
-3	-7	491	505	3	-3	528	495	-10	-5	123	107	-3	-5	340	322
-3	-6	550	571	3	-2	913	936	-10	-4	39	35	-3	-4	251	273
-3	-5	299	299	3	-1	704	691	-10	-3	58	45	-3	-3	278	255
-3	-4	858	866	4	-8	312	301	-10	-2	266	266	-3	-2	109	108
-3	-3	538	539	4	-7	111	103	-10	-1	45	48	-3	-1	745	759
-3	-2	192	183	4	-6	224	223	-9	-6	154	146	-2	-9	110	120
-3	-1	776	801	4	-5	720	683	-9	-5	190	175	-2	-8	234	246
-2	-9	191	202	4	-4	533	546	-9	-4	92	101	-2	-7	526	521
-2	-8	60	67	4	-3	290	313	-9	-3	225	216	-2	-6	283	284
-2	-7	666	662	4	-2	1161	1160	-9	-2	304	315	-2	-5	396	398
-2	-6	424	437	4	-1	795	817	-9	-1	207	202	-2	-4	559	558
-2	-5	178	186	5	-8	362	371	-8	-8	214	226	-2	-3	133	130
-2	-4	754	763	5	-7	293	298	-8	-7	40	41	-2	-2	265	244
-2	-3	533	543	5	-5	480	483	-8	-6	221	215	-2	-1	958	928
-2	-2	52	42	5	-4	370	350	-8	-5	282	270	-1	-10	356	367
-2	-1	664	652	5	-3	69	35	-8	-4	232	235	-1	-9	231	232
-1	-9	277	274	5	-2	520	541	-8	-3	402	390	-1	-8	258	271
-1	-8	43	30	5	-1	540	550	-8	-2	706	678	-1	-7	543	537
-1	-7	414	401	6	-7	172	170	-8	-1	426	424	-1	-6	247	257
-1	-6	405	409	6	-5	269	231	-7	-8	298	302	-1	-5	167	157
-1	-5	296	301	6	-4	365	385	-7	-7	173	171	-1	-4	806	791
-1	-4	416	438	6	-2	220	238	-7	-6	225	231	-1	-3	415	417
-1	-3	929	892	6	-1	424	426	-7	-5	624	613	-1	-2	146	144
				7	-7	163	160	-7	-4	437	448	-1	-1	672	656

Table 42. Continued.

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -1****				6	-5	413	424	-8	-5	299	291	-2	-1	654	660
0	-10	345	348	6	-4	320	320	-8	-4	179	173	-1	-10	216	213
0	-9	237	237	6	-3	296	298	-8	-3	243	241	-1	-9	84	83
0	-8	96	86	6	-2	593	598	-8	-2	338	368	-1	-8	222	226
0	-7	343	341	6	-1	410	410	-8	-1	121	136	-1	-7	457	468
0	-6	308	287	7	-7	196	191	-7	-8	338	337	-1	-6	400	381
0	-5	39	19	7	-6	63	48	-7	-7	91	100	-1	-5	49	49
0	-4	412	399	7	-5	215	216	-7	-6	272	279	-1	-4	451	463
0	-3	1041	1019	7	-4	235	231	-7	-5	604	578	-1	-3	709	706
0	-2	591	568	7	-3	64	56	-7	-4	330	313	-1	-2	654	623
0	-1	981	935	7	-2	155	154	-7	-3	358	338	-1	-1	528	523
1	-9	177	180	7	-1	280	260	-7	-2	1121	1118	0	-10	321	337
1	-7	113	107	8	-7	135	145	-7	-1	338	337	0	-9	210	203
1	-6	344	323	8	-6	80	73	-6	-9	238	233	0	-8	152	147
1	-5	249	265	8	-5	214	208	-6	-8	403	399	0	-7	434	422
1	-4	56	33	8	-4	32	33	-6	-7	313	306	0	-6	526	531
1	-3	496	475	8	-2	56	36	-6	-6	433	436	0	-5	69	38
1	-2	807	805	8	-1	45	40	-6	-5	715	694	0	-4	885	882
1	-1	18	39	9	-5	76	69	-6	-4	369	368	0	-3	1249	1240
2	-9	88	81	9	-4	172	173	-6	-3	395	390	0	-2	309	297
2	-8	110	109	9	-3	76	80	-6	-2	1169	1211	0	-1	870	827
2	-7	41	47	9	-2	102	138	-6	-1	543	529	1	-10	278	266
2	-6	188	203	9	-1	139	146	-5	-9	181	180	1	-9	261	252
2	-5	255	260	10	-5	39	39	-5	-8	429	433	1	-7	351	355
2	-4	222	229	10	-4	315	297	-5	-7	336	334	1	-6	760	742
2	-3	218	239	10	-3	363	367	-5	-6	258	260	1	-5	692	679
2	-2	1086	1069	10	-2	132	118	-5	-5	600	622	1	-4	812	766
2	-1	368	360	10	-1	350	357	-5	-4	527	522	1	-3	1282	1275
3	-9	102	113	11	-4	198	214	-5	-3	308	289	1	-2	1463	1420
3	-8	202	202	11	-3	456	463	-5	-2	606	616	1	-1	634	638
3	-7	115	114	11	-2	124	134	-5	-1	428	423	1	0	883	1214
3	-6	228	205	11	-1	324	317	-4	-8	312	320	2	-10	136	136
3	-5	466	481	12	-1	197	218	-4	-7	224	236	2	-9	231	232
3	-4	371	337	**H = 0****				-4	-6	59	58	2	-8	226	240
3	-3	269	281	-12	-3	348	338	-4	-5	391	385	2	-7	28	23
3	-2	557	571	-12	-2	168	161	-4	-4	286	294	2	-6	528	504
3	-1	153	154	-12	-1	255	230	-4	-3	263	235	2	-5	302	307
4	-9	172	166	-11	-5	65	65	-4	-2	40	44	2	-4	308	291
4	-8	223	196	-11	-4	155	169	-4	-1	507	514	2	-3	802	813
4	-7	32	32	-11	-3	307	271	-3	-10	200	213	2	-2	731	736
4	-6	375	389	-11	-2	265	258	-3	-9	80	79	2	-1	611	592
4	-5	681	698	-11	-1	77	69	-3	-8	187	185	2	0	521	548
4	-4	410	410	-10	-6	98	117	-3	-7	38	38	3	-10	85	88
4	-3	648	651	-10	-5	109	111	-3	-6	105	118	3	-9	143	142
4	-2	950	953	-10	-3	49	41	-3	-5	66	67	3	-8	343	350
4	-1	677	656	-10	-2	293	300	-3	-4	100	68	3	-6	208	203
5	-8	455	459	-10	-1	40	7	-3	-3	82	75	3	-5	310	316
5	-7	282	298	-9	-7	68	76	-3	-2	208	203	3	-4	118	123
5	-6	210	193	-9	-6	138	140	-3	-1	991	1021	3	-3	275	284
5	-5	790	779	-9	-5	237	236	-2	-10	150	142	3	-2	308	308
5	-4	402	370	-9	-4	189	179	-2	-9	111	121	3	-1	90	114
5	-3	392	408	-9	-3	186	137	-2	-8	118	125	3	0	461	471
5	-2	824	854	-9	-2	386	381	-2	-7	203	201	4	-9	124	133
5	-1	145	164	-9	-1	104	93	-2	-5	43	18	4	-8	234	226
6	-8	372	362	-8	-8	197	195	-2	-4	336	336	4	-7	46	35
6	-7	289	288	-8	-7	113	110	-2	-3	232	251	4	-6	326	348
6	-6	306	339	-8	-6	116	120	-2	-2	307	293	4	-5	254	255

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H =		0****		11	-5	59	50	-6	-4	246	221	0	-10	175	193
4	-4	46	15	11	-4	381	364	-6	-3	215	208	0	-9	291	273
4	-3	86	116	11	-3	326	317	-6	-2	371	387	0	-8	163	167
4	-2	240	243	11	-2	58	40	-6	-1	494	504	0	-7	354	366
4	-1	56	60	11	-1	229	236	-6	0	63	54	0	-6	444	447
4	0	287	289	11	0	335	364	-5	-9	271	264	0	-5	136	125
5	-9	252	245	12	-3	435	423	-5	-8	490	476	0	-4	488	495
5	-8	290	293	12	-2	123	134	-5	-7	270	270	0	-3	968	1034
5	-7	100	54	12	-1	294	278	-5	-6	339	341	0	-2	129	127
5	-6	465	424	12	0	444	422	-5	-5	497	518	0	-1	892	863
5	-5	461	476					-5	-4	159	175	0	0	955	890
5	-4	151	138	**H =		1****		-5	-3	146	142	1	-10	350	349
5	-3	199	210	-12	-2	86	74	-5	-2	945	950	1	-9	263	257
5	-2	598	614	-12	-1	207	213	-5	-1	673	698	1	-7	613	615
5	-1	132	132	-12	0	435	436	-5	0	250	255	1	-6	717	714
5	0	37	31	-11	-5	126	137	-5	-10	64	55	1	-5	502	505
6	-9	341	355	-11	-4	322	338	-4	-9	285	285	1	-4	539	555
6	-8	457	452	-11	-3	594	584	-4	-8	481	485	1	-3	1275	1311
6	-7	145	152	-11	-2	223	221	-4	-7	358	368	1	-2	885	985
6	-6	303	330	-11	-1	259	237	-4	-6	355	338	1	-1	765	763
6	-5	680	705	-10	0	524	524	-4	-5	613	624	1	0	1462	1578
6	-4	294	296	-10	-6	318	311	-4	-4	615	589	2	-10	346	342
6	-3	221	220	-10	-5	179	185	-4	-4	208	217	2	-9	352	353
6	-2	565	599	-10	-4	264	255	-4	-3	208	217	2	-8	192	156
6	-1	475	498	-10	-3	524	530	-4	-2	500	521	2	-7	381	350
6	0	208	198	-10	-2	235	239	-4	-1	999	1069	2	-6	893	895
7	-8	401	412	-10	-1	215	209	-4	0	228	263	2	-5	655	630
7	-7	98	99	-10	0	525	532	-3	-10	199	216	2	-4	615	627
7	-6	198	207	-9	-7	109	104	-3	-9	36	31	2	-3	1158	1206
7	-5	363	339	-9	-6	265	254	-3	-8	312	299	2	-2	374	404
7	-4	394	421	-9	-5	223	232	-3	-7	212	220	2	-1	136	124
7	-3	561	545	-9	-4	119	131	-3	-5	416	410	2	0	820	864
7	-2	631	655	-9	-3	405	397	-3	-4	86	97	2	-10	183	186
7	-1	631	655	-9	-2	385	339	-3	-3	96	76	3	-9	388	357
7	0	363	369	-9	-1	127	118	-3	-2	137	137	3	-8	211	223
8	-8	206	209	-9	0	345	335	-3	-1	1301	1448	3	-6	617	596
8	-7	179	159	-8	-8	108	107	-3	0	120	138	3	-5	289	280
8	-6	31	13	-8	-7	83	81	-2	-10	160	154	3	-4	319	302
8	-5	83	110	-8	-6	237	220	-2	-9	115	106	3	-3	655	683
8	-4	391	385	-8	-5	285	289	-2	-8	91	104	3	-2	119	133
8	-3	176	187	-8	-4	117	126	-2	-7	56	50	3	-1	175	167
8	-2	293	295	-8	-3	227	211	-2	-6	57	53	3	0	325	340
8	-1	487	473	-8	-2	40	40	-2	-5	192	169	3	-9	223	221
8	0	465	458	-8	-1	34	1	-2	-4	304	312	4	-8	234	237
9	-7	120	141	-8	0	134	150	-2	-3	631	645	4	-7	71	61
9	-6	131	128	-7	-8	205	189	-2	-2	709	727	4	-6	168	165
9	-5	38	18	-7	-7	78	83	-2	-1	341	344	4	-5	318	331
9	-4	73	80	-7	-6	168	162	-2	0	568	553	4	-4	147	152
9	-3	175	159	-7	-5	286	300	-1	-10	81	90	4	-3	422	432
9	-2	45	31	-7	-3	93	90	-1	-9	46	57	4	-2	153	146
9	-1	156	162	-7	-2	93	94	-1	-7	242	238	4	-1	46	65
9	0	36	55	-7	-1	185	169	-1	-6	133	144	4	0	143	143
10	-6	135	137	-7	0	108	115	-1	-5	169	157	5	-10	84	89
10	-5	106	98	-6	-9	233	226	-1	-4	556	558	5	-9	53	54
10	-4	152	153	-6	-8	313	311	-1	-3	888	966	5	-8	228	214
10	-3	207	208	-6	-7	80	80	-1	-2	372	345	5	-7	166	142
10	-1	283	273	-6	-6	239	233	-1	-1	271	268	5	-6	124	144
10	0	475	421	-6	-5	510	503	-1	0	208	195	5			

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
5	-5	138	127	11	-2	54	84	-6	-1	99	106	0	-7	353	358
5	-4	306	302	11	-1	324	308	-5	-9	246	250	0	-6	520	530
5	-3	221	205	11	0	193	186	-5	-8	176	183	0	-5	160	147
5	-2	325	324	12	-4	338	348	-5	-6	167	151	0	-4	755	790
5	-1	329	328	12	-3	283	292	-5	-5	218	216	0	-3	1099	1096
5	0	244	247	12	-2	28	8	-5	-4	253	256	0	-2	198	178
6	-9	231	250	12	-1	232	218	-5	-3	435	434	0	-1	307	288
6	-8	235	254	12	0	221	229	-5	-2	63	68	0	0	239	227
6	-7	123	123	13	-2	128	114	-5	-1	528	536	1	-11	59	65
6	-6	444	449	13	-1	150	161	-5	0	41	51	1	-10	201	213
6	-5	377	398	13	0	312	316	-4	-9	373	368	1	-9	421	428
6	-4	262	261					-4	-8	406	395	1	-8	43	33
6	-3	47	16	**H =	2****			-4	-7	47	53	1	-7	398	394
6	-2	477	503	-11	-4	185	171	-4	-6	212	213	1	-6	490	501
6	-1	363	389	-11	-3	281	304	-4	-5	495	496	1	-5	41	35
6	0	140	133	-11	-2	84	84	-4	-4	608	593	1	-4	526	520
7	-9	213	211	-11	-1	288	263	-4	-3	123	111	1	-3	158	134
7	-8	342	353	-11	0	391	362	-4	-2	633	661	1	-2	226	227
7	-7	212	223	-10	-6	396	387	-4	-1	610	656	1	-1	856	808
7	-6	331	359	-10	-5	178	180	-4	0	228	223	1	0	739	716
7	-5	475	470	-10	-4	400	364	-3	-10	88	80	2	-10	272	264
7	-4	320	334	-10	-3	537	501	-3	-9	230	235	2	-9	450	444
7	-3	78	76	-10	-2	236	233	-3	-8	453	447	2	-8	142	137
7	-2	388	398	-10	-1	245	259	-3	-7	357	361	2	-7	696	716
7	-1	903	917	-10	0	478	474	-3	-6	93	78	2	-6	707	721
7	0	137	106	-9	-7	243	244	-3	-5	631	618	2	-4	627	682
8	-8	436	452	-9	-6	443	425	-3	-4	657	669	2	-3	1280	1326
8	-7	104	98	-9	-5	248	246	-3	-3	365	376	2	-2	1094	1080
8	-6	33	32	-9	-4	194	182	-3	-2	863	890	2	-1	899	891
8	-5	497	502	-9	-3	482	517	-3	-1	1245	1295	2	0	79	88
8	-4	503	501	-9	-2	317	327	-3	0	665	652	3	-10	443	443
8	-3	267	283	-9	-1	234	204	-2	-10	147	145	3	-9	441	459
8	-2	465	475	-8	0	407	383	-2	-8	292	292	3	-8	263	243
8	-1	894	897	-8	-8	167	184	-2	-7	441	432	3	-7	621	611
8	0	450	440	-8	-7	164	169	-2	-6	223	224	3	-6	722	748
9	-8	211	200	-8	-6	374	365	-2	-5	390	395	3	-5	111	108
9	-7	243	249	-8	-5	127	140	-2	-4	678	700	3	-4	191	230
9	-6	138	138	-8	-4	62	22	-2	-3	524	521	3	-3	552	569
9	-5	109	102	-8	-3	777	742	-2	-2	155	153	3	-2	285	263
9	-4	463	452	-8	-1	50	55	-2	-1	1561	1644	3	-1	234	224
9	-3	323	311	-8	0	99	123	-2	0	514	511	3	0	729	717
9	-2	240	242	-7	-8	267	247	-1	-11	103	110	4	-10	297	297
9	-1	447	434	-7	-7	77	73	-1	-10	100	98	4	-9	434	426
9	0	156	146	-7	-6	224	224	-1	-9	45	44	4	-8	145	135
10	-7	171	164	-7	-5	263	249	-1	-8	114	121	4	-7	316	332
10	-6	83	77	-7	-4	88	79	-1	-7	303	310	4	-6	474	478
10	-5	56	45	-7	-3	63	35	-1	-6	396	403	4	-5	238	245
10	-4	208	215	-7	-2	49	37	-1	-5	159	145	4	-4	141	145
10	-3	164	166	-7	-1	47	39	-1	-4	747	781	4	-3	217	244
10	-2	175	154	-7	0	25	18	-1	-3	468	486	4	-2	634	652
10	-1	328	324	-6	-9	158	158	-1	-2	246	218	4	-1	118	118
10	0	108	99	-6	-8	78	77	-1	-1	1257	1245	4	0	436	436
11	-6	164	155	-6	-7	97	91	-1	0	455	453	5	-10	80	80
11	-5	77	51	-6	-6	186	168	0	-11	34	30	5	-9	299	286
11	-4	171	155	-6	-5	115	131	0	-10	104	89	5	-8	50	35
11	-3	232	221	-6	-4	160	156	0	-9	206	227	5	-7	88	81
				-6	-2	118	119	0	-8	139	137	5	-6	85	80

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H =	2****			11	-2	244	239	-5	-3	94	93	0	-4	555	545
5	-5	110	109	11	-1	178	146	-5	-2	421	415	0	-3	528	506
5	-3	233	233	11	0	310	281	-5	-1	306	315	0	-2	57	39
5	-2	401	406	12	-5	36	19	-5	0	249	236	0	-1	188	189
5	-1	541	553	12	-4	159	162	-4	-10	44	37	0	0	208	195
5	0	58	58	12	-3	161	134	-4	-9	77	83	1	-11	29	13
6	-10	60	52	12	-2	119	99	-4	-8	200	196	1	-10	244	244
6	-9	85	102	12	-1	107	109	-4	-7	222	177	1	-9	221	226
6	-8	87	80	12	0	95	102	-4	-6	200	182	1	-8	101	103
6	-7	72	51	13	-3	148	146	-4	-5	445	450	1	-7	270	262
6	-6	75	85	13	-2	80	92	-4	-4	386	411	1	-6	278	260
6	-5	176	184	13	-1	114	116	-4	-3	99	104	1	-5	108	98
6	-4	358	361	13	0	224	216	-4	-2	789	774	1	-4	79	80
6	-3	92	65	**H =	3****			-4	-1	576	607	1	-3	407	371
6	-2	449	466	-10	-5	79	69	-4	0	45	28	1	-2	526	510
6	-1	373	392	-10	-4	221	226	-3	-10	43	52	1	-1	215	206
6	0	60	64	-10	-3	276	271	-3	-9	182	194	1	0	151	147
7	-9	55	45	-10	-2	68	60	-3	-8	425	419	2	-11	36	31
7	-8	178	159	-10	-1	248	242	-3	-7	257	266	2	-10	299	292
7	-7	140	150	-10	0	272	264	-3	-6	125	121	2	-9	152	142
7	-6	80	81	-9	-6	449	452	-3	-5	794	806	2	-8	113	114
7	-5	358	357	-9	-5	117	97	-3	-4	1007	1046	2	-7	336	351
7	-4	449	468	-9	-4	297	285	-3	-3	155	118	2	-6	105	103
7	-3	103	105	-9	-3	246	256	-3	-2	674	711	2	-5	233	221
7	-2	657	665	-9	-2	158	163	-3	-1	898	929	2	-4	775	769
7	-1	451	467	-9	-1	137	165	-3	0	228	220	2	-3	261	252
7	0	52	34	-9	0	402	395	-2	-11	259	269	2	-2	915	895
8	-9	89	76	-8	-7	248	251	-2	-10	334	318	2	-1	265	267
8	-8	285	325	-8	-6	358	352	-2	-9	162	161	2	0	296	298
8	-7	338	316	-8	-5	114	134	-2	-8	586	583	3	-11	92	74
8	-6	215	190	-8	-4	274	280	-2	-7	711	731	3	-10	283	296
8	-5	521	538	-8	-3	429	421	-2	-6	249	237	3	-9	419	408
8	-4	509	518	-8	-2	426	406	-2	-5	728	750	3	-8	251	233
8	-3	32	41	-8	0	397	392	-2	-4	896	941	3	-7	395	410
8	-2	645	684	-7	-8	130	135	-2	-3	318	311	3	-6	519	548
8	-1	655	682	-7	-7	130	126	-2	-2	991	1021	3	-5	225	202
8	0	64	72	-7	-6	249	252	-2	-1	1409	1432	3	-4	410	383
9	-8	349	320	-7	-5	279	238	-2	0	458	446	3	-3	1070	1095
9	-7	353	368	-7	-4	58	58	-1	-11	207	208	3	-2	225	220
9	-5	575	568	-7	-3	358	348	-1	-10	344	346	3	-1	122	118
9	-4	652	662	-7	-2	253	243	-1	-9	86	81	3	0	950	948
9	-3	46	48	-7	-1	106	95	-1	-8	383	377	4	-11	60	60
9	-2	505	506	-7	0	79	84	-1	-7	613	620	4	-10	331	331
9	-1	790	785	-6	-9	143	137	-1	-6	97	106	4	-9	418	416
9	0	168	136	-6	-8	145	136	-1	-5	202	231	4	-8	100	111
10	-7	393	403	-6	-7	49	47	-1	-4	793	817	4	-7	520	553
10	-6	187	175	-6	-6	173	158	-1	-3	427	423	4	-6	656	687
10	-5	333	341	-6	-5	56	35	-1	-2	565	552	4	-5	370	375
10	-4	532	526	-6	-4	59	71	-1	-1	598	602	4	-4	116	119
10	-3	186	164	-6	-3	36	24	-1	0	293	281	4	-3	802	833
10	-2	220	237	-6	-2	213	205	0	-11	227	232	4	-2	663	677
10	-1	263	285	-6	-1	133	141	0	-10	111	119	4	-1	285	270
10	0	54	61	-6	0	51	29	0	-9	276	266	4	0	959	994
11	-6	82	88	-5	-9	67	63	0	-8	159	145	5	-10	242	226
11	-5	73	91	-5	-6	92	88	0	-7	397	395	5	-9	298	317
11	-4	175	160	-5	-5	101	95	0	-6	315	323	5	-8	223	223
11	-3	45	28	-5	-4	122	101	0	-5	215	218	5	-7	202	210

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	3****		11	-7	391	376	-6	-1	113	105	0	-9	82	76
5	-6	396	414	11	-6	81	61	-6	0	358	347	0	-8	478	488
5	-5	552	596	11	-5	273	284	-5	-9	171	161	0	-7	488	500
5	-4	140	147	11	-4	331	331	-5	-8	143	150	0	-6	89	92
5	-3	331	369	11	-3	77	82	-5	-7	106	93	0	-5	386	379
5	-2	819	888	11	-2	239	222	-5	-6	121	117	0	-4	426	433
5	-1	252	252	11	-1	250	243	-5	-5	149	150	0	-3	110	101
5	0	618	629	11	0	274	273	-5	-4	202	170	0	-2	43	51
6	-10	35	52	12	-6	32	43	-5	-3	342	337	0	-1	490	475
6	-9	203	187	12	-5	53	35	-5	-2	474	466	0	0	649	629
6	-8	112	156	12	-4	123	101	-5	-1	82	75	1	-11	198	188
6	-7	264	266	12	-3	151	142	-5	0	263	275	1	-10	175	184
6	-6	85	89	12	-2	107	95	-4	-10	78	79	1	-9	121	128
6	-5	366	392	12	-1	57	43	-4	-9	44	46	1	-8	188	193
6	-4	63	78	12	0	241	233	-4	-8	201	195	1	-7	334	329
6	-3	42	38	13	-4	53	35	-4	-7	167	151	1	-6	32	26
6	-2	681	706	13	-3	121	129	-4	-5	377	378	1	-5	73	69
6	-1	412	401	13	-2	87	96	-4	-4	332	328	1	-4	165	173
6	0	304	328	13	-1	43	37	-4	-3	250	239	1	-3	149	151
7	-9	79	83	13	0	109	108	-4	-2	626	618	1	-2	79	63
7	-8	73	64		**H =	4****		-4	-1	288	270	1	-1	265	262
7	-7	208	215	-13	0	128	152	-4	0	237	221	1	0	654	643
7	-6	50	34	-10	-3	48	51	-3	-10	171	170	2	-11	91	84
7	-5	308	294	-10	-1	33	30	-3	-8	270	259	2	-10	156	172
7	-4	388	397	-10	0	56	58	-3	-7	279	268	2	-9	139	142
7	-3	184	204	-9	-6	116	143	-3	-6	172	168	2	-8	39	32
7	-2	291	306	-9	-5	34	29	-3	-5	666	660	2	-7	191	184
7	-1	130	142	-9	-4	114	104	-3	-4	526	534	2	-6	181	181
7	0	318	332	-9	-3	164	143	-3	-3	47	59	2	-4	261	230
8	-8	287	299	-9	-2	137	132	-3	-2	457	469	2	-3	186	194
8	-7	248	256	-9	-1	97	91	-3	-1	127	149	2	-2	283	268
8	-6	31	30	-9	0	145	149	-3	0	53	50	2	-1	79	75
8	-5	418	432	-8	-7	284	283	-2	-11	322	310	2	0	530	529
8	-4	282	285	-8	-6	391	377	-2	-10	173	167	3	-11	38	47
8	-3	260	264	-8	-5	45	32	-2	-9	150	136	3	-10	220	206
8	-2	530	533	-8	-4	46	58	-2	-8	501	509	3	-9	61	63
8	-1	391	385	-8	-3	270	293	-2	-7	588	572	3	-8	78	51
8	0	90	86	-8	-2	302	315	-2	-5	845	865	3	-7	68	60
9	-9	127	121	-8	-1	31	26	-2	-4	636	685	3	-6	140	143
9	-8	357	380	-8	0	439	435	-2	-3	105	103	3	-5	283	282
9	-7	295	259	-7	-8	57	53	-2	-2	495	508	3	-4	55	41
9	-6	245	231	-7	-7	244	236	-2	-1	636	649	3	-3	1181	1171
9	-5	596	614	-7	-6	252	269	-2	0	405	395	3	-2	786	778
9	-4	362	344	-7	-5	199	215	-1	-11	340	324	3	-1	513	509
9	-3	68	70	-7	-4	119	125	-1	-10	408	397	3	0	828	830
9	-2	723	727	-7	-3	541	510	-1	-9	150	131	4	-11	102	90
9	-1	508	528	-7	-2	538	537	-1	-8	582	582	4	-10	285	320
9	0	66	68	-7	-1	100	78	-1	-7	666	676	4	-9	270	276
10	-8	389	381	-7	0	644	660	-1	-6	62	27	4	-8	128	140
10	-7	451	452	-6	-9	277	279	-1	-5	844	858	4	-7	349	361
10	-6	118	117	-6	-8	106	114	-1	-4	651	662	4	-6	600	616
10	-5	622	607	-6	-7	83	91	-1	-3	262	272	4	-5	795	799
10	-4	633	633	-6	-6	311	305	-1	-2	431	424	4	-4	311	297
10	-3	205	185	-6	-5	593	555	-1	-1	557	547	4	-3	1103	1113
10	-2	363	364	-6	-4	32	15	-1	0	505	501	4	-2	831	819
10	-1	567	571	-6	-3	356	365	0	-11	281	280	4	-1	201	201
10	0	153	147	-6	-2	572	581	0	-10	448	429	4	0	758	791

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	4****		10	-4	378	402	-6	-2	604	617	0	-9	71	72
5	-10	195	197	10	-3	78	75	-6	-1	63	53	0	-8	622	619
5	-9	431	455	10	-2	252	221	-6	0	552	545	0	-7	481	489
5	-8	212	206	10	-1	583	600	-5	-9	329	323	0	-6	50	45
5	-7	408	420	10	0	359	355	-5	-8	347	343	0	-5	555	556
5	-6	683	695	11	-8	355	361	-5	-7	73	33	0	-4	825	820
5	-5	645	655	11	-7	372	360	-5	-6	603	577	0	-3	518	529
5	-4	151	164	11	-6	61	71	-5	-5	503	507	0	-2	430	415
5	-3	1020	1039	11	-5	470	480	-5	-3	499	506	0	-1	469	500
5	-2	838	882	11	-4	532	512	-5	-2	518	525	0	0	572	573
5	-1	86	68	11	-3	362	350	-5	-1	226	209	1	-11	370	374
5	0	940	980	11	-2	174	183	-5	0	387	388	1	-10	393	378
6	-10	146	141	11	-1	560	570	-4	-10	30	25	1	-9	139	134
6	-9	378	407	11	0	435	440	-4	-9	225	225	1	-8	590	591
6	-8	377	354	12	-7	319	331	-4	-8	326	326	1	-7	295	297
6	-7	121	92	12	-6	174	159	-4	-7	113	118	1	-6	248	236
6	-6	558	586	12	-5	191	196	-4	-6	267	279	1	-5	529	510
6	-5	554	576	12	-4	305	316	-4	-5	317	302	1	-4	769	754
6	-4	129	125	12	-3	187	201	-4	-4	140	138	1	-3	538	535
6	-3	865	908	12	-2	33	21	-4	-3	249	254	1	-2	153	126
6	-2	710	736	12	-1	291	296	-4	-2	462	443	1	-1	823	814
6	-1	200	176	12	0	413	414	-4	-1	221	219	1	0	810	813
6	0	549	568	13	-5	50	47	-4	0	120	113	2	-11	171	171
7	-10	35	18	13	-4	178	181	-3	-10	128	128	2	-10	316	307
7	-9	191	175	13	-3	243	219	-3	-8	280	279	2	-9	46	36
7	-8	249	258	13	-2	128	128	-3	-7	117	119	2	-8	289	282
7	-6	313	327	13	-1	225	235	-3	-5	241	240	2	-7	407	417
7	-5	427	417	13	0	204	187	-3	-4	141	118	2	-6	452	445
7	-4	107	103		**H =	5****		-3	-3	59	58	2	-5	305	310
7	-3	263	291	-13	-2	283	289	-3	-2	394	373	2	-4	503	496
7	-2	236	240	-13	-1	37	35	-3	-1	100	97	2	-3	149	187
7	-1	318	300	-13	0	201	200	-3	0	38	51	2	-2	301	293
7	0	182	183	-9	-4	48	67	-2	-10	275	270	2	-1	541	543
8	-10	71	59	-9	-3	73	81	-2	-9	40	43	2	0	293	303
8	-9	100	79	-9	-1	50	43	-2	-8	321	317	3	-11	43	39
8	-8	206	213	-9	0	158	155	-2	-7	99	104	3	-10	90	86
8	-7	123	124	-8	-6	163	163	-2	-6	61	61	3	-9	68	55
8	-6	36	40	-8	-5	136	119	-2	-5	271	273	3	-8	64	76
8	-5	277	288	-8	-4	92	92	-2	-4	330	315	3	-7	92	90
8	-4	30	27	-8	-3	239	229	-2	-3	131	121	3	-6	77	78
8	-3	323	306	-8	-2	101	100	-2	-2	50	55	3	-5	205	181
8	-2	120	115	-8	-1	54	52	-2	-1	237	244	3	-4	120	134
8	-1	68	48	-8	0	210	202	-2	0	30	13	3	-3	248	265
9	-9	65	61	-7	-7	179	173	-1	-11	260	258	3	-2	160	143
9	-8	268	267	-7	-6	274	292	-1	-10	273	258	3	-1	269	284
9	-7	151	156	-7	-5	94	108	-1	-9	117	112	3	0	781	766
9	-6	66	63	-7	-4	149	150	-1	-8	427	434	4	-10	104	97
9	-5	306	300	-7	-3	421	423	-1	-7	456	452	4	-9	65	48
9	-4	125	113	-7	-2	340	332	-1	-6	156	154	4	-8	148	143
9	-3	165	175	-7	-1	132	121	-1	-5	400	404	4	-7	66	59
9	-2	196	198	-7	0	512	519	-1	-4	431	439	4	-6	441	438
9	-1	277	275	-6	-8	155	156	-1	-3	51	48	4	-5	331	354
9	0	84	95	-6	-7	282	276	-1	-2	332	325	4	-4	108	96
10	-8	310	310	-6	-6	562	564	-1	-1	563	558	4	-3	670	688
10	-7	246	259	-6	-5	567	552	-1	0	222	241	4	-2	225	215
10	-6	95	104	-6	-4	70	68	0	-11	471	448	4	-1	149	171
10	-5	395	391	-6	-3	593	585	0	-10	403	397	4	0	587	576



Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	
5	-10	140	127	10	-5	48	45	-5	-4	121	109	0	-1	825	835	
5	-9	226	231	10	-4	102	98	-5	-3	545	557	0	0	483	502	
5	-8	344	345	10	-3	54	63	-5	-2	504	514	1	-11	319	318	
5	-7	39	52	10	-2	82	78	-5	-1	39	40	1	-10	221	232	
5	-6	65.1	640	10	-1	175	178	-5	0	304	301	1	-9	63	51	
5	-5	436	443	11	-8	194	183	-4	-9	440	444	1	-8	330	331	
5	-4	462	472	11	-7	76	76	-4	-8	555	536	1	-7	482	483	
5	-3	634	641	11	-6	28	26	-4	-6	606	595	1	-6	138	151	
5	-2	598	587	11	-5	116	107	-4	-5	510	527	1	-5	279	279	
5	-1	373	373	11	-4	361	357	-4	-4	61	63	1	-4	968	951	
5	0	437	436	11	-3	276	271	-4	-3	364	352	1	-3	604	591	
6	-11	138	147	11	-2	210	219	-4	-2	308	304	1	-2	307	303	
6	-10	169	177	11	-1	465	450	-4	-1	162	162	1	-1	933	934	
6	-9	483	489	11	0	342	347	-4	0	63	64	1	0	707	695	
6	-8	437	431	12	-7	305	302	-3	-10	79	78	2	-11	259	266	
6	-7	213	222	12	-6	239	229	-3	-9	354	344	2	-10	315	317	
6	-6	805	818	12	-5	84	90	-3	-8	328	325	2	-9	164	152	
6	-5	548	560	12	-4	422	438	-3	-7	33	37	2	-8	300	284	
6	-4	193	198	12	-4	422	438	-3	-6	297	304	2	-7	650	647	
6	-3	849	881	12	-3	268	266	-3	-6	297	304	2	-7	650	647	
6	-3	849	881	12	-3	268	266	-3	-5	230	226	2	-6	551	533	
6	-2	767	766	12	-2	171	155	-3	-4	30	36	2	-5	47	46	
6	-1	53	46	12	-1	473	481	-3	-4	30	36	2	-5	47	46	
6	0	601	608	12	0	306	319	-3	-3	187	184	2	-4	968	968	
7	-10	147	147	12	-1	473	481	-3	-2	179	177	2	-3	952	941	
7	-9	430	456	13	-5	190	179	-3	-1	184	162	2	-2	132	129	
7	-8	522	522	13	-4	475	475	-3	0	56	59	2	-1	789	792	
7	-7	141	135	13	-3	292	275	-2	-9	165	159	2	0	517	542	
7	-6	827	852	13	-2	24	27	-2	-8	98	103	3	-11	81	83	
7	-5	556	578	13	-1	434	429	-2	-7	49	50	3	-10	252	252	
7	-4	48	27	13	0	381	369	-2	-6	189	179	3	-9	363	353	
7	-3	624	622	13	-13	-2	250	240	-2	-5	108	86	3	-8	156	155
7	-2	769	793	13	-2	190	179	-2	-4	67	55	3	-7	481	482	
7	-1	156	152	13	-1	61	42	-2	-3	47	42	3	-6	661	677	
7	0	464	440	13	-8	102	107	-2	-2	79	63	3	-5	65	54	
8	-9	299	315	13	-8	212	213	-2	-1	197	199	3	-4	690	681	
8	-8	383	379	13	-2	83	79	-2	0	99	102	3	-3	555	546	
8	-7	88	84	13	-8	170	159	-1	-11	125	123	3	-2	30	30	
8	-6	535	556	13	-7	209	186	-1	-10	45	36	3	-1	507	514	
8	-5	362	352	13	-7	102	97	-1	-9	120	118	3	0	196	203	
8	-4	173	169	13	-7	102	97	-1	-8	120	118	3	0	196	203	
8	-3	245	253	13	-4	140	146	-1	-8	132	135	4	-11	49	48	
8	-2	280	275	13	-3	358	358	-1	-7	41	22	4	-10	156	163	
8	-1	52	38	13	-2	77	89	-1	-6	28	13	4	-9	326	314	
9	0	30	46	13	-1	129	132	-1	-5	74	45	4	-7	279	281	
9	-9	172	175	13	-7	146	132	-1	-4	171	157	4	-6	217	232	
9	-8	283	284	13	-6	155	141	-1	-3	29	24	4	-5	34	44	
9	-6	140	128	13	-6	155	141	-1	-2	141	147	4	-4	198	169	
9	-5	154	165	13	-6	324	350	-1	-1	360	336	4	-3	286	305	
9	-4	37	26	13	-6	291	296	-1	0	169	160	4	-2	97	92	
9	-3	120	131	13	-6	172	160	0	-11	211	221	4	-1	358	363	
9	-2	92	77	13	-6	502	497	0	-10	72	77	4	0	262	247	
9	-1	220	221	13	-6	332	341	0	-9	37	31	5	-11	66	57	
9	0	106	117	13	-6	128	132	0	-8	210	205	5	-10	158	159	
10	-9	65	88	13	-6	0	374	372	0	-7	234	227	5	-9	196	174
10	-8	210	197	13	-5	392	391	0	-6	141	121	5	-8	37	18	
10	-6	33	3	13	-5	224	229	0	-5	217	232	5	-7	274	297	
				13	-4	19	130	0	-4	536	539	5	-6	331	300	
				13	-3	71	666	0	-3	347	331	5	-5	264	287	
				13	-2	5	631	0	-2	238	246	5	-4	527	535	



Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	6****		11	-8	79	86	-3	-4	38	42	K	L	FOBS	FCAL
5	-3	299	277	11	-7	108	97	-3	-3	141	141	2	-1	788	788
5	-2	44	47	11	-6	29	26	-3	-2	420	426	2	0	517	529
5	-1	186	184	11	-5	72	81	-3	-1	268	273	3	-11	254	240
5	0	243	255	11	-4	208	215	-3	0	118	119	3	-10	347	351
6	-11	87	71	11	-3	28	25	-2	-10	30	23	3	-9	133	122
6	-10	203	184	11	-2	125	130	-2	-9	299	282	3	-8	261	270
6	-9	421	427	11	-1	229	232	-2	-8	219	228	3	-7	758	749
6	-8	64	68	11	0	52	51	-2	-6	163	161	3	-6	532	522
6	-7	168	168	12	-7	209	198	-2	-5	293	291	3	-5	338	333
6	-6	515	518	12	-6	64	62	-2	-4	276	278	3	-4	926	919
6	-5	132	108	12	-5	150	160	-2	-3	73	63	3	-3	678	685
6	-4	463	471	12	-4	320	315	-2	-2	323	316	3	-2	182	182
6	-3	369	359	12	-3	151	161	-2	-1	330	325	3	-1	469	462
6	-2	187	210	12	-2	381	402	-1	-9	191	184	3	0	320	319
6	-1	28	23	12	-1	328	302	-1	-8	99	106	4	-11	103	99
6	0	280	276	12	0	138	147	-1	-7	140	138	4	-10	335	348
7	-10	270	288	13	-6	108	90	-1	-6	55	43	4	-9	413	423
7	-9	549	543	13	-5	215	218	-1	-5	157	142	4	-8	29	27
7	-8	190	185	13	-4	443	461	-1	-4	253	251	4	-7	496	478
7	-7	186	203	13	-3	181	171	-1	-3	36	24	4	-6	312	318
7	-6	540	554	13	-2	281	287	-1	-2	237	241	4	-5	223	215
7	-5	336	317	13	-1	420	416	-1	-1	207	201	4	-4	443	470
7	-4	230	197	13	0	219	226	-1	0	80	80	4	-3	282	282
7	-3	634	643		**H =	7****		0	-11	117	115	4	-2	299	299
7	-2	674	678	-7	-4	182	191	0	-9	99	104	4	-1	202	197
7	-1	259	257	-7	-3	180	183	0	-8	73	70	4	0	350	355
7	0	339	332	-6	-6	136	134	0	-7	233	233	5	-10	115	120
8	-10	158	155	-6	-5	68	73	0	-6	99	103	5	-9	228	212
8	-9	382	367	-6	-4	146	147	0	-5	162	160	5	-8	120	132
8	-8	327	338	-6	-3	119	128	0	-4	144	150	5	-7	498	511
8	-7	107	115	-6	-2	65	61	0	-3	234	235	5	-6	126	125
8	-6	541	537	-6	-1	56	51	0	-2	363	363	5	-5	69	54
8	-5	545	549	-6	0	117	131	0	-1	318	315	5	-4	198	201
8	-4	310	301	-5	-8	30	37	0	0	29	24	5	-3	207	200
8	-3	208	209	-5	-7	191	188	1	-11	211	218	5	-2	96	81
8	-2	642	663	-5	-6	293	298	1	-10	125	129	5	-1	76	76
8	-1	386	393	-5	-5	160	151	1	-9	68	66	5	0	131	115
8	0	55	43	-5	-4	83	89	1	-8	217	224	6	-10	131	137
9	-10	73	71	-5	-3	340	338	1	-7	348	356	6	-9	242	242
9	-9	243	250	-5	-2	332	346	1	-6	90	90	6	-8	71	79
9	-8	259	273	-5	-1	30	42	1	-5	323	308	6	-7	166	151
9	-7	158	136	-5	0	155	146	1	-4	641	643	6	-6	295	303
9	-6	172	162	-4	-9	396	401	1	-3	318	310	6	-5	67	46
9	-5	350	358	-4	-8	245	236	1	-2	438	438	6	-3	106	106
9	-4	206	199	-4	-7	63	67	1	-1	648	650	6	-2	105	91
9	-3	55	72	-4	-6	496	487	1	0	343	337	6	-1	89	102
9	-2	356	375	-4	-5	365	366	2	-11	296	297	6	0	170	168
9	-1	384	376	-4	-3	323	317	2	-10	293	303	7	-10	216	229
10	-9	57	57	-4	-2	430	423	2	-9	67	78	7	-9	353	343
10	-8	86	80	-4	-1	229	226	2	-8	226	232	7	-8	142	136
10	-7	228	248	-4	0	244	239	2	-7	578	556	7	-7	195	203
10	-5	162	145	-3	-9	389	384	2	-6	297	307	7	-6	301	294
10	-4	189	201	-3	-8	379	361	2	-5	455	450	7	-5	202	200
10	-3	198	179	-3	-7	150	133	2	-4	841	833	7	-4	91	102
10	-2	86	80	-3	-6	340	341	2	-3	361	354	7	-3	221	185
10	-1	241	238	-3	-5	437	440	2	-2	283	291	7	-2	415	404
													-1	291	295

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 7****				**H = 8****											
7	0	357	372	-5	-6	40	31	1	-8	156	151	6	-10	201	190
8	-10	204	229	-5	-4	33	30	1	-7	191	189	6	-9	131	146
8	-9	461	444	-5	-3	35	38	1	-6	41	38	6	-8	138	156
8	-8	202	190	-5	-2	41	48	1	-5	200	210	6	-7	216	220
8	-7	116	105	-5	-1	78	79	1	-4	161	156	6	-6	74	59
8	-6	328	327	-5	0	95	97	1	-3	83	91	6	-5	243	278
8	-5	536	540	-4	-7	36	49	1	-2	212	217	6	-4	133	142
8	-4	125	116	-4	-6	108	111	1	-1	214	222	6	-3	348	341
8	-3	328	316	-4	-5	145	140	1	0	60	67	6	-2	226	226
8	-2	745	771	-4	-4	63	43	2	-11	78	88	6	-1	99	91
8	-1	434	460	-4	-3	239	240	2	-10	301	300	6	0	220	220
8	0	277	271	-4	-2	298	294	2	-9	93	101	7	-10	60	53
9	-10	101	102	-4	-1	84	92	2	-8	259	259	7	-9	80	94
9	-9	374	374	-4	0	89	95	2	-7	365	381	7	-8	77	78
9	-8	312	315	-3	-9	256	268	2	-6	122	103	7	-7	30	25
9	-7	42	6	-3	-8	281	268	2	-5	225	218	7	-6	181	210
9	-6	260	271	-3	-7	82	80	2	-4	277	276	7	-5	121	93
9	-5	506	493	-3	-6	335	335	2	-3	72	78	7	-4	203	220
9	-4	418	448	-3	-5	381	375	2	-2	218	223	7	-3	221	225
9	-3	410	418	-3	-4	160	155	2	-1	353	324	7	-2	113	123
9	-2	629	617	-3	-3	333	337	2	0	113	109	7	-1	32	45
9	-1	449	454	-3	-2	534	537	3	-11	285	291	7	0	122	102
9	0	191	190	-3	-1	227	234	3	-10	385	371	8	-10	89	87
10	-9	160	165	-3	0	176	174	3	-9	70	69	8	-9	93	88
10	-8	228	231	-2	-9	346	337	3	-8	371	363	8	-8	181	188
10	-7	154	151	-2	-8	311	307	3	-7	641	627	8	-7	42	30
10	-6	82	77	-2	-6	329	323	3	-6	182	155	8	-6	152	141
10	-5	380	374	-2	-5	532	538	3	-5	410	408	8	-5	174	159
10	-4	245	241	-2	-4	252	249	3	-4	543	533	8	-4	134	146
10	-3	80	81	-2	-3	263	256	3	-3	435	403	8	-3	147	164
10	-2	444	451	-2	-2	530	527	3	-1	543	536	8	-2	209	205
10	-1	241	265	-2	-1	463	453	3	0	437	425	8	-1	40	24
10	0	228	239	-2	0	299	308	4	-11	340	350	8	0	270	282
11	-8	84	90	-1	-9	186	190	4	-10	546	539	9	-9	220	218
11	-7	189	199	-1	-8	244	241	4	-9	242	242	9	-8	261	257
11	-6	32	42	-1	-7	148	145	4	-8	290	302	9	-7	39	38
11	-5	246	258	-1	-6	213	222	4	-7	594	571	9	-6	286	283
11	-4	131	116	-1	-5	590	589	4	-6	493	501	9	-5	550	564
11	-3	42	61	-1	-4	357	350	4	-5	402	405	9	-4	120	109
11	-2	270	290	-1	-3	184	188	4	-4	572	546	9	-3	338	333
11	-1	62	61	-1	-2	523	542	4	-3	614	602	9	-2	547	547
11	0	195	199	-1	-1	449	459	4	-2	48	51	9	-1	318	317
12	-7	112	118	-1	0	125	123	4	-1	437	431	9	0	188	192
12	-5	203	195	0	-10	50	57	4	0	590	579	10	-9	334	354
12	-4	135	135	0	-9	65	65	5	-11	148	148	10	-8	394	387
12	-3	102	104	0	-8	212	222	5	-10	492	491	10	-7	181	174
12	-2	165	156	0	-7	286	283	5	-9	249	233	10	-6	228	224
12	-1	124	121	0	-6	95	93	5	-8	183	168	10	-5	576	579
12	0	73	78	0	-5	359	352	5	-7	548	559	10	-4	201	196
13	-6	116	106	0	-4	210	224	5	-6	293	275	10	-3	400	413
13	-5	195	197	0	-3	105	100	5	-5	72	66	10	-2	420	420
13	-4	323	334	0	-2	189	180	5	-4	403	403	10	-1	244	254
13	-3	24	12	0	-1	74	78	5	-3	499	506	10	0	182	156
13	-2	170	164	0	0	92	110	5	-2	240	234	11	-8	360	356
13	-1	141	160	1	-10	159	156	5	-1	199	174	11	-7	181	183
13	0	45	48	1	-9	89	90	5	0	476	476	11	-6	253	269
								6	-11	36	38	11	-5	456	457

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 8****				0	-1	233	220	6	-9	227	223	12	-7	126	134
11	-4	286	297	0	0	96	90	6	-8	52	56	12	-6	203	212
11	-3	245	252	1	-10	148	149	6	-7	220	217	12	-5	311	313
11	-2	403	386	1	-9	96	103	6	-6	433	444	12	-4	217	228
11	-1	298	298	1	-8	289	263	6	-5	102	91	12	-3	113	105
11	0	26	16	1	-7	297	296	6	-4	214	211	12	-2	237	248
12	-7	122	121	1	-6	191	200	6	-3	527	530	12	-1	236	232
12	-6	153	148	1	-5	402	387	6	-2	536	542	13	-4	148	168
12	-5	287	292	1	-4	246	233	6	-1	171	166	13	-3	36	26
12	-4	111	107	1	-3	190	191	6	0	495	490	**H = 10****			
12	-3	78	74	1	-2	174	173	7	-10	153	173	-2	-6	275	262
12	-2	245	247	1	-1	46	53	7	-9	147	153	-2	-5	221	222
12	-1	143	150	1	0	76	81	7	-8	97	90	-2	-4	109	106
13	-5	186	184	2	-10	167	157	7	-6	331	333	-2	-3	203	213
13	-4	76	76	2	-9	30	32	7	-5	334	340	-2	-2	107	119
13	-2	58	55	2	-8	268	271	7	-4	71	77	-1	-8	267	267
13	-1	101	111	2	-7	60	60	7	-3	396	400	-1	-7	71	75
**H = 9****				2	-6	48	48	7	-2	345	334	-1	-6	351	351
-4	-6	40	39	2	-5	231	226	7	-1	75	67	-1	-5	301	303
-4	-5	60	53	2	-4	137	141	7	0	288	288	-1	-4	57	44
-4	-3	88	93	2	-3	239	230	8	-10	81	75	-1	-3	258	255
-4	-2	94	98	2	-2	118	101	8	-9	71	71	-1	-2	241	248
-3	-7	32	25	2	-1	80	78	8	-8	202	211	-1	-1	147	140
-3	-6	108	108	2	0	93	75	8	-6	135	126	0	-8	396	396
-3	-5	183	189	3	-10	227	238	8	-5	198	214	0	-7	63	66
-3	-4	55	48	3	-9	62	63	8	-4	46	46	0	-6	325	321
-3	-3	234	233	3	-8	337	337	8	-3	222	201	0	-5	364	360
-3	-2	238	245	3	-7	138	130	8	-2	100	97	0	-4	121	119
-3	-1	38	26	3	-6	56	63	8	-1	315	323	0	-3	153	171
-3	0	177	177	3	-5	225	228	8	0	184	161	0	-2	494	495
-2	-8	313	315	3	-4	186	170	9	-9	104	109	0	-1	297	303
-2	-7	50	64	3	-3	75	56	9	-8	156	151	0	0	31	30
-2	-6	238	242	3	-2	59	62	9	-7	85	82	1	-9	210	214
-2	-5	367	367	3	-1	184	190	9	-6	326	325	1	-8	477	493
-2	-4	206	196	3	0	208	211	9	-5	114	100	1	-7	169	157
-2	-3	307	306	4	-10	289	282	9	-3	359	363	1	-6	252	246
-2	-2	464	463	4	-8	291	293	9	-2	245	253	1	-5	371	383
-2	-1	88	69	4	-7	406	412	9	-1	123	135	1	-4	336	336
-2	0	86	95	4	-6	100	75	9	0	198	190	1	-3	72	66
-1	-9	280	277	4	-5	137	127	9	-9	284	279	1	-2	266	255
-1	-8	435	437	4	-4	370	365	10	-8	343	339	1	-1	218	216
-1	-7	92	94	4	-3	359	374	10	-7	44	32	1	0	126	118
-1	-6	320	329	4	-2	95	93	10	-6	391	398	2	-9	55	61
-1	-5	526	530	4	-1	337	327	10	-5	342	343	2	-8	253	243
-1	-4	387	377	4	0	464	455	10	-3	371	373	2	-7	191	185
-1	-3	317	324	5	-10	460	467	10	-2	329	322	2	-6	187	185
-1	-2	625	632	5	-9	241	242	10	-1	43	18	2	-5	110	123
-1	-1	432	449	5	-8	85	76	10	0	258	251	2	-4	156	141
-1	0	120	118	5	-7	508	503	11	-8	407	408	2	-3	106	98
0	-9	188	186	5	-6	466	457	11	-7	92	91	2	-2	113	121
0	-8	476	475	5	-5	30	40	11	-6	356	348	2	-1	269	262
0	-7	262	266	5	-4	318	322	11	-5	493	505	2	0	151	150
0	-6	208	208	5	-3	466	458	11	-4	77	55	3	-10	116	114
0	-5	608	608	5	-2	344	342	11	-3	247	235	3	-9	74	91
0	-4	439	421	5	-1	309	329	11	-2	337	346	3	-8	123	121
0	-3	127	106	5	0	665	667	11	-1	176	174	3	-7	130	141
0	-2	458	452	6	-10	316	307	11	0	33	23	3	-5	40	37

Table 42. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 10****															
3	-4	215	208	8	-4	266	253	2	-2	259	258	8	-7	444	438
3	-3	215	200	8	-3	237	247	2	-1	396	401	8	-6	412	403
3	-2	28	22	8	-2	63	71	3	-8	224	243	8	-5	56	50
3	-1	190	189	8	-1	110	92	3	-7	162	146	8	-4	313	313
3	0	163	173	8	0	152	157	3	-6	32	37	8	-3	423	413
4	-10	101	101	9	-9	142	156	3	-5	167	175	8	-2	164	158
4	-8	162	154	9	-8	111	116	3	-4	205	220	8	-1	148	149
4	-7	75	71	9	-7	83	105	3	-3	191	196	9	-8	119	129
4	-6	166	171	9	-6	190	181	3	-2	160	162	9	-7	253	259
4	-5	46	47	9	-5	115	109	3	-1	294	295	9	-6	303	307
4	-4	302	291	9	-4	174	177	3	0	123	135	9	-5	90	98
4	-3	272	260	9	-3	93	106	4	-8	73	71	9	-4	153	154
4	-2	45	21	9	-2	51	51	4	-7	152	160	9	-3	187	175
4	-1	240	236	9	0	45	54	4	-6	93	104	9	-2	97	100
4	0	201	183	10	-8	79	69	4	-5	75	67	9	-1	47	43
5	-10	247	250	10	-7	115	120	4	-4	146	143	10	-7	132	115
5	-9	131	123	10	-6	236	230	4	-3	205	205	10	-6	80	89
5	-8	162	161	10	-5	100	111	4	-2	75	71	10	-5	41	44
5	-7	310	302	10	-4	83	76	4	-1	160	167	10	-4	100	94
5	-6	331	333	10	-3	176	170	4	0	28	19	10	-3	137	141
5	-5	149	130	10	-2	203	216	5	-9	76	77	10	-2	84	76
5	-4	417	398	10	-1	122	112	5	-8	82	82	11	-5	103	115
5	-3	408	420	10	0	95	92	5	-7	159	161	11	-4	126	127
5	-2	120	125	11	-7	29	12	5	-6	170	160	**H = 12****			
5	-1	327	323	11	-6	305	291	5	-4	178	191	3	-6	81	78
5	0	415	430	11	-5	319	313	5	-3	169	163	3	-5	328	325
6	-10	304	292	11	-4	123	121	5	-2	62	54	3	-4	343	344
6	-9	288	286	11	-3	55	61	5	-1	164	165	4	-7	228	231
6	-7	464	472	11	-2	250	262	5	0	34	25	4	-6	48	46
6	-6	360	342	11	-1	124	124	6	-9	169	161	4	-5	231	220
6	-5	114	123	12	-5	321	324	6	-8	45	50	4	-4	317	321
6	-4	491	486	12	-4	160	172	6	-7	321	305	4	-3	76	75
6	-3	462	461	12	-3	63	55	6	-6	338	341	5	-7	141	145
6	-2	79	92	12	-2	326	328	6	-5	53	14	5	-6	31	25
6	-1	342	327	**H = 11****				6	-4	335	342	5	-5	171	174
6	0	434	435	0	-6	202	199	6	-3	233	223	5	-4	175	170
7	-9	321	335	0	-5	247	237	6	-2	89	89	5	-3	53	61
7	-7	236	230	0	-4	57	53	6	-1	235	234	6	-7	150	157
7	-6	454	455	0	-3	122	131	6	0	228	234	6	-6	58	50
7	-5	100	92	1	-7	122	119	7	-9	358	359	6	-5	128	118
7	-4	333	329	1	-6	218	225	7	-8	59	68	6	-4	145	135
7	-3	432	419	1	-5	435	437	7	-7	456	444	7	-7	232	228
7	-2	176	190	1	-4	280	286	7	-6	366	370	7	-6	159	153
7	-1	205	214	1	-3	29	16	7	-5	48	56	7	-5	114	112
7	0	307	317	1	-2	376	375	7	-4	372	366	7	-4	250	262
8	-9	187	172	2	-8	349	358	7	-3	434	428	7	-3	112	116
8	-8	131	144	2	-7	209	211	7	-2	46	36	8	-6	299	300
8	-7	84	80	2	-6	83	81	7	-1	201	199	8	-4	215	212
8	-6	361	377	2	-5	340	318	7	0	303	298	8	-3	289	296
8	-5	126	113	2	-4	332	335	8	-8	35	23	9	-5	178	180

Table 43. 10\*(Fobs vs. Fcal) For [Rh2C12(mu-SO2)(DPM)2].

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -20****				**H = -18****				**H = -17****				**H = -16****			
0	2	432	404	3	5	138	153	3	13	646	633	2	15	770	788
0	4	904	926	3	9	416	413	3	14	148	136	2	16	221	229
0	6	1016	1023	3	11	459	466	4	0	262	319	3	5	390	435
0	8	756	806	3	12	234	226	4	2	138	125	3	7	827	827
0	10	504	502	4	0	305	310	4	4	148	176	3	8	264	268
1	1	216	210	4	4	118	89	4	6	288	327	3	9	811	878
1	6	152	122	4	7	205	183	4	7	219	222	3	10	304	306
1	7	122	129	4	11	310	305	4	8	286	284	3	11	686	675
1	8	231	246	5	0	415	406	4	9	278	313	3	12	238	210
1	9	385	333	5	1	245	255	4	11	363	351	3	13	463	480
1	10	278	281	5	2	365	354	4	13	240	268	3	15	275	254
1	11	327	321	5	3	210	156	5	0	163	147	3	16	204	190
2	1	510	491	5	4	361	358	5	1	142	128	4	2	202	216
2	3	290	273	5	6	469	480	5	2	180	197	4	5	206	220
2	6	271	243	5	7	140	160	5	4	233	179	4	8	323	280
2	7	144	155	5	8	377	411	5	6	195	163	4	9	423	429
2	8	326	314	5	10	196	228	5	9	147	182	4	10	330	368
2	9	325	309	6	6	121	93	5	11	127	124	4	11	480	455
2	10	203	160	6	7	101	29	5	13	263	251	4	12	176	200
3	2	222	200	0	0	566	544	6	0	330	342	4	13	482	512
3	7	240	209	0	2	1242	1215	6	2	393	417	4	14	138	98
3	9	152	115	0	4	1908	1931	6	4	419	438	4	15	468	436
4	4	402	420	0	6	1519	1543	6	6	455	456	5	0	273	321
4	5	310	313	0	8	1118	1073	6	7	121	94	5	1	136	143
4	6	337	322	0	10	531	616	6	8	413	430	5	2	387	411
4	7	231	249	0	12	213	230	6	9	297	263	5	3	327	341
**H = -19****				0	12	213	230	6	10	342	352	5	4	513	505
0	0	135	106	1	0	214	207	6	11	218	206	5	5	314	343
0	2	282	263	1	2	193	200	7	7	113	97	5	6	635	656
0	6	304	297	1	5	179	131	**H = -17****				5	7	290	318
0	8	525	489	1	6	282	242	0	0	385	401	5	8	413	394
0	10	333	319	1	7	242	252	0	2	305	285	5	9	236	219
0	12	262	258	1	8	341	320	0	12	191	203	5	11	265	275
1	0	168	166	1	9	336	323	0	14	409	386	5	12	250	180
1	1	447	483	1	10	271	280	0	16	650	661	5	13	251	239
1	1	447	483	1	11	359	370	1	0	587	623	5	14	163	187
1	2	509	483	1	13	459	446	1	1	272	276	6	0	211	200
1	4	964	986	1	14	286	273	1	2	1288	1328	6	2	173	210
1	6	985	964	1	15	543	541	1	4	1408	1423	6	4	265	257
1	7	184	171	2	1	405	424	1	5	373	323	6	6	182	162
1	8	776	779	2	2	157	148	1	6	1169	1175	7	0	315	317
1	9	276	241	2	3	158	120	1	7	261	238	7	1	113	56
1	10	410	415	2	4	387	386	1	8	891	872	7	2	357	358
1	11	363	370	2	5	167	197	1	9	458	457	7	4	398	404
1	12	137	92	2	6	480	498	1	10	315	283	7	5	289	341
1	13	481	501	2	7	504	513	1	11	578	560	7	6	437	423
2	1	300	284	2	8	323	320	1	13	549	531	7	7	429	412
2	8	250	246	2	9	636	673	1	15	184	202	7	8	452	454
2	9	277	325	2	11	623	622	2	1	242	193	7	9	606	576
2	10	406	408	2	12	144	154	2	4	184	169	7	10	343	328
2	11	578	585	2	13	701	687	2	5	184	190	7	11	571	603
2	12	240	238	2	15	340	353	2	7	214	263	8	7	246	215
2	13	676	673	3	0	221	235	2	9	488	474	8	9	189	168
3	0	298	272	3	5	138	188	2	11	579	576	8	10	216	220
3	1	375	398	3	9	321	331	2	12	367	387	**H = -16****			
3	2	327	299	3	11	613	628	2	13	813	864	0	0	1314	1278
3	3	148	139	3	12	146	101	2	14	374	357	0	2	1794	1836

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -16****															
0	4	1422	1423	4	14	173	184	1	0	1061	1046	4	17	205	185
0	6	991	966	4	15	238	222	1	2	950	955	4	18	530	505
0	8	663	607	4	17	179	178	1	3	242	211	5	0	942	935
0	10	207	224	5	0	330	336	1	4	715	742	5	1	697	747
0	14	302	260	5	2	555	473	1	6	649	686	5	2	1081	1160
0	16	156	120	5	4	244	286	1	7	281	274	5	3	861	831
1	0	484	510	5	8	329	357	1	8	223	273	5	4	1213	1241
1	1	201	177	5	10	148	154	1	9	555	491	5	5	945	965
1	5	285	287	5	12	203	251	1	11	435	398	5	6	676	642
1	6	203	178	5	13	356	363	1	12	308	301	5	7	538	555
1	8	298	258	5	14	512	542	1	14	288	354	5	9	388	410
1	10	214	158	5	15	168	180	1	15	223	166	5	10	217	232
1	11	357	318	5	16	683	733	1	16	434	410	5	11	420	353
1	12	369	404	6	0	836	838	1	18	366	351	5	12	237	185
1	13	534	535	6	2	918	899	2	0	209	124	5	13	159	160
1	14	412	448	6	3	186	203	2	3	304	346	5	16	170	152
1	15	501	475	6	4	858	874	2	4	180	185	5	17	139	118
1	16	617	564	6	6	606	575	2	9	375	323	6	0	630	635
1	17	186	180	6	8	209	226	2	10	673	669	6	2	382	407
1	18	474	511	6	9	185	195	2	11	687	667	6	4	218	204
2	0	246	213	6	12	421	422	2	12	536	565	6	5	188	190
2	2	460	481	6	14	437	423	2	13	675	637	6	7	312	312
2	3	255	237	7	0	196	232	2	14	315	368	6	8	213	258
2	4	463	452	7	5	221	241	2	15	382	397	6	9	422	471
2	5	679	724	7	7	142	144	2	16	431	390	6	11	162	203
2	6	446	398	7	8	148	127	2	18	574	553	6	12	528	538
2	7	623	654	7	9	285	298	3	0	178	216	6	14	930	926
2	9	796	788	7	10	241	266	3	1	181	126	6	16	981	947
2	11	722	769	7	11	325	262	3	3	476	469	7	0	872	853
2	13	456	436	7	13	225	198	3	4	247	229	7	2	853	877
2	15	172	120	7	14	360	373	3	5	1028	1011	7	3	361	327
2	16	152	119	8	1	160	186	3	6	268	199	7	4	608	575
3	3	256	272	8	3	266	251	3	7	1141	1109	7	5	603	581
3	5	292	221	8	4	283	266	3	8	458	408	7	6	501	557
3	7	288	271	8	5	410	410	3	9	861	815	7	7	774	815
3	8	344	333	8	6	465	439	3	11	482	500	7	8	211	208
3	9	789	784	8	7	664	646	3	13	442	470	7	9	736	735
3	10	767	777	8	8	375	381	3	14	232	149	7	11	513	438
3	11	839	838	8	9	772	762	3	15	279	342	7	12	433	419
3	12	562	575	8	10	141	155	3	16	175	191	7	13	201	230
3	13	782	757	8	11	619	645	3	18	182	165	7	14	237	279
3	14	207	191	9	1	159	155	4	0	307	315	8	1	165	175
3	15	591	648	9	3	159	80	4	1	246	226	8	4	273	280
3	17	536	476	9	6	196	189	4	2	282	288	8	5	424	408
4	1	242	284	9	7	272	257	4	3	358	329	8	6	350	349
4	2	443	391	9	8	279	266	4	5	186	211	8	7	423	470
4	3	509	495	9	9	374	381	4	6	506	509	8	8	302	281
4	4	604	606	9	10	248	210	4	7	307	255	8	8	661	625
4	5	846	820	**H = -15****				4	8	461	434	8	9	244	235
4	6	639	653	0	0	862	835	4	9	656	677	8	10	573	586
4	7	1028	983	0	2	202	164	4	10	296	297	8	11	455	478
4	8	326	398	0	6	360	382	4	11	581	628	8	13	128	151
4	9	711	731	0	8	524	547	4	12	258	198	9	0	473	479
4	10	227	217	0	12	531	478	4	13	655	567	9	1	287	301
4	11	569	537	0	14	525	621	4	14	524	485	9	2	222	178
4	13	343	385	0	16	632	634	4	15	425	411	9	5	221	189
				0	18	463	472	4	16	455	436	9	7	484	490

Table 43: Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -15****															
9	9	592	660	4	7	1111	1071	9	11	506	487	3	6	498	413
9	11	389	407	4	9	869	920	9	13	369	362	3	7	1224	1262
9	12	151	139	4	11	478	511	10	0	588	616	3	8	396	404
10	0	163	157	4	13	467	406	10	1	133	85	3	9	895	873
10	7	283	265	5	0	691	691	10	2	420	417	3	11	616	640
10	9	409	421	5	2	408	421	10	4	138	123	3	13	612	580
**H = -14****															
0	0	546	678	5	3	214	187	10	5	274	278	3	14	437	421
0	2	429	357	5	6	501	546	10	7	363	381	3	15	326	259
0	6	253	195	5	7	396	402	10	9	300	296	3	18	176	112
0	10	283	316	5	10	542	485	10	11	238	280	4	0	404	448
0	12	918	910	5	11	229	269	11	0	140	136	4	1	252	200
0	14	681	817	5	12	858	820	11	2	127	103	4	2	233	250
0	16	558	579	5	13	514	460	11	7	201	189	4	3	191	129
0	18	388	401	5	14	1050	1029	11	8	120	110	4	5	229	268
1	0	225	234	5	15	200	208	**H = -13****				4	7	460	445
1	8	198	222	5	16	1005	1032	0	4	288	348	4	8	333	346
1	9	268	241	6	18	935	903	0	12	508	545	4	9	758	710
1	10	332	406	6	0	1575	1569	0	14	927	851	4	10	364	441
1	12	444	314	6	1	474	477	0	16	512	556	4	11	635	715
1	14	597	562	6	2	1509	1519	0	18	466	475	4	12	638	698
1	16	541	605	6	4	1085	1037	0	20	255	275	4	13	436	552
1	17	168	152	6	6	340	330	1	0	260	238	4	14	750	725
1	18	521	511	6	7	502	481	1	1	588	571	4	15	534	499
2	1	285	280	6	8	329	270	1	2	411	397	4	16	675	626
2	2	307	311	6	9	365	376	1	3	525	547	4	18	488	403
2	3	658	732	6	10	518	511	1	4	509	554	4	19	378	381
2	4	598	603	6	11	238	206	1	5	323	329	5	0	1364	1394
2	5	630	634	6	12	514	491	1	6	385	414	5	1	418	471
2	6	506	537	6	13	381	299	1	7	673	646	5	2	1727	1624
2	7	563	537	6	14	244	235	1	8	188	154	5	3	594	633
2	8	201	205	7	0	471	391	1	9	502	538	5	4	853	898
2	9	678	700	7	5	267	288	1	10	475	464	5	5	569	528
2	11	552	535	7	7	494	474	1	12	1185	1126	5	7	558	557
2	12	192	202	7	9	781	745	1	13	315	291	5	8	441	458
2	14	590	632	7	10	189	45	1	14	1015	1018	5	10	289	251
2	15	217	203	7	11	494	492	1	15	215	276	5	14	414	362
2	16	571	574	7	12	631	610	1	16	388	405	5	16	249	266
2	18	263	192	7	13	242	318	1	19	211	154	6	0	569	650
3	3	337	358	7	14	845	806	1	20	197	230	6	5	294	281
3	7	616	622	7	15	243	243	2	2	230	318	6	7	706	743
3	8	221	314	7	16	630	641	2	4	322	308	6	9	305	329
3	9	885	848	8	0	268	211	2	6	365	348	6	10	515	509
3	10	425	342	8	1	339	412	2	7	249	191	6	12	904	894
3	11	609	621	8	2	289	355	2	11	360	355	6	14	1070	983
3	13	486	455	8	3	676	683	2	12	284	288	6	16	956	930
3	15	388	379	8	5	708	700	2	14	652	553	6	18	726	718
3	18	201	194	8	7	1007	1069	2	16	544	601	7	0	938	893
3	19	468	484	8	9	1153	1137	2	17	287	284	7	1	543	540
4	0	714	740	8	11	664	636	2	18	390	448	7	2	756	764
4	1	517	503	8	13	230	221	2	19	549	555	7	3	532	494
4	2	1063	1043	9	3	216	144	2	20	149	181	7	4	590	488
4	3	851	869	9	4	332	337	3	0	465	436	7	5	991	939
4	4	996	1013	9	5	405	436	3	1	598	616	7	7	1233	1220
4	5	1186	1228	9	6	357	349	3	2	235	249	7	9	941	906
4	6	268	231	9	7	626	622	3	3	1267	1204	7	10	440	498
				9	9	755	771	3	4	413	379	7	11	656	661
				9	10	144	119	3	5	1633	1622	7	12	405	356

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -13****															
7	13	453	400	1	11	253	261	5	10	689	643	10	0	599	624
7	14	186	198	1	12	845	916	5	11	717	732	10	1	569	519
8	0	155	13	1	14	1221	1142	5	12	766	683	10	2	521	509
8	1	198	237	1	15	416	397	5	13	387	435	10	3	733	704
8	2	200	196	1	16	894	858	5	14	931	967	10	5	670	644
8	4	196	65	1	18	458	427	5	15	502	497	10	7	720	706
8	5	282	308	1	19	413	386	5	16	1149	1105	10	8	421	356
8	7	693	631	2	0	760	750	5	18	725	698	10	9	480	472
8	9	805	800	2	1	1192	1168	6	0	1297	1255	10	10	544	565
8	10	391	382	2	2	955	981	6	1	341	275	10	11	413	380
8	11	544	522	2	3	1170	1158	6	2	1000	954	10	12	386	377
8	12	497	400	2	4	1251	1286	6	4	433	383	10	13	153	131
8	13	211	228	2	5	1429	1369	6	5	389	464	10	14	268	262
8	14	410	385	2	6	764	748	6	7	233	269	11	0	390	358
9	0	376	330	2	7	1263	1253	6	8	590	533	11	1	335	293
9	1	353	435	2	8	451	414	6	9	616	560	11	2	186	193
9	2	231	202	2	9	818	867	6	10	688	639	11	3	227	154
9	3	549	565	2	12	704	679	6	11	751	746	11	6	176	192
9	5	659	734	2	13	523	401	6	12	300	255	11	7	235	213
9	6	247	166	2	14	700	676	6	14	420	366	11	8	207	228
9	7	971	941	2	18	368	371	7	1	430	412	11	10	382	396
9	9	954	897	2	19	202	205	7	3	271	223	11	11	164	146
9	10	246	252	2	20	425	409	7	4	193	88	12	0	343	355
9	11	694	698	3	1	256	226	7	5	243	193	12	2	355	347
9	12	260	240	3	2	181	148	7	7	503	562	12	3	135	183
9	13	255	255	3	3	241	183	7	9	461	393	12	5	186	219
10	0	183	193	3	4	488	524	7	10	577	551	12	6	219	236
10	1	147	145	3	5	588	552	7	11	475	483	12	7	133	102
10	5	260	274	3	6	660	638	7	12	644	734	12	8	431	432
10	7	411	436	3	7	593	640	7	13	241	275	**H = -11****			
10	9	400	363	3	8	353	286	7	14	791	810	0	4	540	550
10	12	326	319	3	9	484	458	7	16	494	507	0	6	878	949
11	0	481	487	3	10	515	423	8	0	233	256	0	8	315	357
11	2	569	573	3	11	716	651	8	1	1047	999	0	10	1788	1796
11	3	181	134	3	12	321	345	8	3	907	892	0	12	1970	2019
11	4	201	182	3	13	422	500	8	5	1133	1030	0	14	1513	1575
11	6	154	181	3	17	438	459	8	6	338	345	0	16	739	737
11	7	176	183	3	19	774	755	8	7	1370	1259	0	18	622	555
11	8	180	208	4	0	1095	1009	8	8	227	196	1	0	949	929
11	10	248	232	4	1	562	516	8	9	1167	1207	1	1	1047	1071
12	3	158	136	4	2	784	778	8	11	794	727	1	2	859	874
12	4	147	173	4	3	1350	1298	8	12	277	213	1	3	804	861
12	5	119	133	4	4	578	569	8	13	260	249	1	4	366	408
**H = -12****															
0	2	282	187	4	6	578	569	8	14	213	219	1	5	1084	1129
0	6	232	135	4	7	1361	1364	8	16	203	218	1	6	392	426
0	8	652	701	4	8	671	705	9	0	318	317	1	7	958	1011
0	10	1072	1173	4	9	1056	931	9	2	389	350	1	8	560	509
0	12	1362	1348	4	10	381	435	9	4	299	250	1	9	256	208
0	14	950	861	4	14	275	219	9	5	395	371	1	10	597	625
0	18	223	188	4	16	240	216	9	7	594	596	1	11	291	311
0	20	384	334	4	18	181	152	9	8	521	567	1	12	557	589
1	5	221	264	4	20	169	123	9	9	472	432	1	13	278	241
1	6	264	205	5	0	597	634	9	10	209	220	1	14	296	279
1	9	364	350	5	5	243	221	9	11	282	253	1	17	251	189
1	10	554	539	5	6	392	396	9	13	169	153	1	18	314	313
				5	8	482	507	9	14	232	193	1	19	225	241
				5	9	432	337	9	15	369	393	1	20	336	336



Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -11****															
1	21	322	313	5	3	424	489	9	3	1258	1176	1	15	578	521
2	0	512	471	5	5	627	559	9	4	457	418	1	16	578	567
2	2	268	204	5	6	546	541	9	5	1333	1277	1	17	461	479
2	4	566	593	5	7	684	656	9	6	387	345	1	18	306	280
2	7	445	380	5	8	284	362	9	7	1092	1061	1	19	596	622
2	8	268	279	5	9	253	286	9	9	841	842	1	21	662	656
2	9	638	642	5	10	483	437	9	10	341	351	2	0	1695	1717
2	10	538	544	5	11	648	577	9	11	490	448	2	1	1776	1793
2	12	688	733	5	12	461	475	9	12	188	62	2	2	1169	1133
2	13	251	201	5	13	467	412	9	14	171	169	2	3	2189	2188
2	14	848	817	5	14	544	612	9	16	219	219	2	5	2074	2010
2	15	522	467	5	16	258	246	10	0	312	299	2	6	197	94
2	16	588	501	5	17	303	252	10	1	427	395	2	7	2015	1907
2	17	743	731	6	0	335	216	10	2	379	383	2	9	397	332
2	19	1040	991	6	1	482	380	10	4	302	254	2	11	217	64
2	20	207	224	6	5	351	348	10	5	241	239	2	17	340	267
2	21	871	869	6	6	326	266	10	7	336	299	2	19	249	331
3	0	532	514	6	9	259	185	10	10	500	518	2	21	513	451
3	1	1615	1671	6	10	525	543	10	12	630	645	3	0	608	578
3	2	583	546	6	12	570	594	10	13	303	278	3	1	260	306
3	3	2179	2256	6	14	676	688	10	14	519	513	3	2	545	488
3	4	564	617	6	15	331	262	11	0	790	721	3	3	326	340
3	5	2113	2116	6	16	880	815	11	1	208	181	3	4	695	755
3	6	590	619	6	17	254	215	11	2	533	508	3	5	603	676
3	7	1552	1513	6	18	617	635	11	3	170	209	3	6	250	280
3	8	866	909	6	19	155	144	11	6	682	600	3	7	317	324
3	9	836	809	7	0	494	482	11	8	764	791	3	10	255	106
3	10	326	280	7	1	486	536	11	10	663	663	3	15	557	553
3	11	333	363	7	3	384	351	11	12	538	511	3	16	277	298
3	13	397	253	7	4	272	41	12	0	367	376	3	17	1118	1068
3	18	333	324	7	5	489	463	12	5	151	166	3	18	498	466
3	19	320	306	7	6	356	399	12	8	222	217	3	19	920	901
3	20	188	182	7	7	648	607	12	9	158	125	3	20	202	220
4	0	376	345	7	8	688	587	12	10	453	451	3	21	626	650
4	1	282	289	7	9	817	812	13	1	472	432	4	0	986	954
4	2	306	284	7	10	665	673	13	2	226	226	4	1	1510	1475
4	3	364	364	7	11	404	483	13	3	684	623	4	2	284	173
4	4	742	725	7	12	324	371	13	5	472	461	4	3	1620	1586
4	5	308	298	7	14	325	217	**H = -10****				4	4	402	389
4	6	786	770	7	16	305	267	0	0	1158	1129	4	5	1329	1351
4	7	587	579	7	17	227	173	0	2	603	603	4	6	899	901
4	8	736	732	7	18	158	112	0	6	1159	1055	4	7	828	863
4	9	566	587	8	1	552	538	0	8	812	871	4	8	980	967
4	10	723	667	8	3	218	213	0	10	892	915	4	9	395	397
4	11	916	762	8	6	487	502	0	16	401	338	4	10	786	786
4	12	444	517	8	7	510	556	0	20	235	254	4	12	739	713
4	13	599	618	8	8	428	379	1	0	370	322	4	13	245	232
4	14	807	767	8	9	518	489	1	1	249	261	4	14	517	463
4	15	216	258	8	10	529	549	1	2	282	255	4	15	297	215
4	16	713	752	8	12	300	359	1	3	373	356	4	17	265	291
4	17	400	377	8	13	248	270	1	4	656	599	4	19	318	345
4	18	381	427	8	14	321	301	1	7	832	830	5	4	210	245
4	19	393	451	8	15	379	376	1	8	931	995	5	6	534	575
5	0	1224	1233	8	16	265	279	1	9	805	839	5	7	311	314
5	1	201	59	8	17	343	345	1	10	2054	2037	5	8	461	409
5	2	873	900	9	1	1113	1053	1	12	2218	2238	5	9	348	340
				9	2	478	393	1	14	1334	1377	5	11	458	371

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -10****															
5	12	408	427	10	2	459	512	1	10	744	705	4	17	769	771
5	13	265	287	10	3	989	1024	1	11	246	218	4	18	213	165
5	14	766	686	10	4	262	280	1	12	549	461	4	19	591	591
5	16	627	609	10	5	763	778	1	13	279	281	4	21	514	492
5	18	193	225	10	6	389	463	1	14	341	347	5	0	874	773
6	0	395	330	10	7	444	477	1	16	574	527	5	1	220	285
6	1	209	157	10	8	873	904	1	21	398	422	5	3	547	567
6	3	381	265	10	9	390	404	2	1	493	551	5	4	435	513
6	6	290	327	10	10	588	578	2	2	233	235	5	5	420	450
6	8	461	525	10	11	191	189	2	3	1065	1008	5	6	733	706
6	9	328	272	10	12	188	221	2	5	1112	1074	5	8	535	433
6	10	461	423	10	13	167	128	2	6	809	793	5	10	838	944
6	11	512	462	10	15	219	195	2	7	775	772	5	12	1209	1203
6	12	248	267	11	0	241	271	2	8	905	881	5	14	394	346
6	14	302	339	11	1	347	345	2	10	912	857	5	15	218	217
6	16	285	234	11	2	249	255	2	11	259	303	5	17	204	231
7	1	762	750	11	4	283	237	2	12	1102	1085	5	18	223	186
7	2	336	286	11	6	415	394	2	13	341	350	5	19	201	273
7	3	362	376	11	7	189	187	2	14	370	332	6	1	456	360
7	5	356	333	11	8	513	488	2	15	744	718	6	3	245	125
7	7	441	475	11	10	701	655	2	17	911	966	6	4	216	161
7	9	286	283	11	12	772	795	2	18	352	382	6	6	234	318
7	10	704	686	12	0	623	604	2	19	1046	1006	6	7	226	238
7	11	199	139	12	1	407	376	2	20	198	196	6	8	373	364
7	12	892	864	12	2	195	153	2	21	828	824	6	9	232	117
7	13	430	346	12	3	551	568	3	0	285	265	6	12	677	663
7	14	493	477	12	4	418	398	3	1	2768	2739	6	13	172	197
7	15	405	452	12	5	581	598	3	3	2544	2610	6	14	600	639
7	16	446	473	12	6	696	708	3	4	555	599	6	15	352	358
7	17	406	426	12	7	436	487	3	5	1488	1490	6	16	508	530
7	18	413	431	12	8	711	721	3	6	287	257	6	17	364	358
8	1	563	628	12	9	212	211	3	7	1354	1342	6	20	258	230
8	2	216	135	12	10	589	541	3	8	904	895	7	2	195	143
8	3	566	556	13	1	296	305	3	9	497	558	7	5	260	283
8	4	355	349	13	3	160	130	3	10	483	476	7	6	426	437
8	5	813	871	13	4	160	168	3	12	240	269	7	8	758	766
8	6	444	465	13	5	348	392	3	13	425	548	7	10	617	658
8	7	631	572	13	7	358	290	3	15	640	572	7	12	240	266
8	8	658	616	**H = -9****				3	17	237	216	7	15	237	263
8	9	376	384	0	2	458	521	3	18	233	207	7	16	224	276
8	10	457	395	0	4	815	789	3	19	281	279	7	17	217	279
8	12	344	392	0	6	425	435	3	20	209	194	8	1	443	536
8	14	354	315	0	8	1702	1664	3	21	348	312	8	2	201	145
8	16	279	292	0	10	2762	2895	4	1	195	60	8	3	316	238
8	17	302	305	0	12	2635	2591	4	2	432	405	8	7	438	462
8	18	147	79	0	14	1595	1565	4	3	524	450	8	8	214	196
9	1	270	313	0	16	745	759	4	4	449	504	8	9	307	349
9	2	289	306	0	18	413	361	4	5	375	354	8	10	562	458
9	6	443	437	1	0	581	587	4	6	803	717	8	12	524	520
9	7	269	250	1	1	1700	1631	4	7	209	211	8	13	424	392
9	9	252	261	1	2	226	283	4	9	493	519	8	14	313	359
9	12	221	196	1	3	1165	1315	4	10	218	249	8	15	627	601
9	13	511	522	1	4	866	953	4	11	267	270	8	16	262	268
9	15	678	678	1	5	1572	1633	4	12	406	362	8	17	758	804
10	0	604	623	1	6	1367	1328	4	14	666	702	9	0	207	178
10	1	1056	1042	1	7	1031	1054	4	15	635	618	9	1	1165	1175
				1	8	1050	1071	4	16	399	474	9	3	1149	1211

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -9****				1	1	454	467	4	0	742	865	7	11	216	185
9	5	1051	1019	1	2	251	215	4	1	1612	1724	7	12	936	902
9	6	467	571	1	4	596	555	4	2	246	245	7	13	534	583
9	7	738	756	1	5	382	388	4	3	1409	1394	7	14	456	489
9	9	419	375	1	6	589	657	4	4	716	763	7	15	741	781
9	15	190	169	1	7	1033	1015	4	5	1112	1068	7	16	315	327
9	17	215	260	1	8	1158	1193	4	6	933	936	7	17	841	799
10	1	233	221	1	9	686	629	4	7	215	214	7	19	391	436
10	2	248	306	1	10	2008	2067	4	8	1318	1396	8	1	438	423
10	4	211	174	1	11	337	271	4	10	1308	1334	8	3	587	595
10	5	344	405	1	12	1872	1901	4	11	496	427	8	4	323	300
10	6	369	326	1	14	903	945	4	12	636	657	8	5	543	541
10	7	288	357	1	15	550	491	4	13	790	819	8	6	227	80
10	8	660	645	1	16	582	603	4	14	337	275	8	7	186	170
10	9	264	286	1	17	612	642	4	16	390	402	8	8	521	604
10	10	407	398	1	19	650	711	4	17	319	345	8	10	473	460
10	12	343	367	1	21	579	555	4	18	231	221	8	12	286	304
10	13	293	257	1	22	236	263	4	19	301	306	8	13	213	113
10	14	150	167	2	0	535	476	4	21	191	218	8	16	300	294
10	15	595	620	2	1	1916	1915	5	1	306	326	8	17	228	213
10	16	181	187	2	2	1351	1285	5	3	417	393	8	18	264	288
11	0	813	767	2	3	2102	2101	5	4	425	342	9	1	240	205
11	4	588	630	2	4	1607	1623	5	5	544	516	9	5	441	491
11	6	908	913	2	5	2075	2061	5	6	232	296	9	6	366	292
11	7	319	269	2	6	887	907	5	8	298	311	9	7	398	393
11	8	861	839	2	7	916	983	5	9	499	512	9	8	420	339
11	10	639	693	2	8	644	632	5	10	839	699	9	9	340	320
11	12	443	427	2	9	218	127	5	11	589	609	9	13	496	503
11	13	146	88	2	10	866	825	5	12	954	971	9	14	242	303
12	0	175	186	2	11	362	446	5	13	521	582	9	15	631	626
12	2	172	160	2	12	632	666	5	14	524	539	9	17	814	819
12	3	242	185	2	13	224	203	5	16	212	79	10	1	1042	1026
12	5	238	188	2	14	517	481	5	17	201	251	10	2	196	243
12	6	275	291	2	15	307	293	5	18	162	227	10	3	846	800
12	8	522	511	2	16	311	333	5	19	450	424	10	4	712	713
12	10	641	644	2	17	240	144	5	20	412	403	10	5	753	700
12	12	630	659	2	18	410	406	6	0	237	117	10	6	966	935
13	0	265	244	2	19	272	293	6	3	253	126	10	7	559	520
13	1	943	934	2	20	265	281	6	4	571	597	10	8	699	743
13	3	881	898	2	21	520	504	6	5	620	676	10	9	259	339
13	4	317	339	3	0	599	626	6	6	920	868	10	10	610	581
13	5	580	568	3	2	537	536	6	7	272	202	10	12	298	295
13	6	412	417	3	3	335	287	6	8	1038	991	10	13	148	185
13	7	431	453	3	5	260	245	6	10	1032	1056	10	15	207	181
13	8	490	501	3	6	449	386	6	11	341	250	11	1	220	83
13	9	272	308	3	7	511	452	6	12	883	822	11	2	256	213
**H = -8****				3	9	563	557	6	15	187	105	11	3	269	258
0	0	954	997	3	10	172	28	6	19	166	99	11	4	416	455
0	2	188	47	3	11	634	642	6	20	149	168	11	5	451	420
0	4	960	940	3	13	718	661	7	0	218	248	11	6	617	606
0	6	1385	1519	3	14	408	397	7	3	326	286	11	7	260	248
0	8	1370	1391	3	15	1140	1122	7	4	233	151	11	8	506	522
0	10	655	752	3	16	425	456	7	5	473	445	11	9	506	509
0	12	850	828	3	17	949	1001	7	7	721	777	11	10	510	536
0	14	1044	1025	3	18	431	420	7	8	563	582	11	11	281	266
0	16	955	942	3	19	944	917	7	9	277	373	11	12	618	645
0	22	184	138	3	21	708	724	7	10	905	997	11	14	496	514

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -8****				2	7	164	102	5	11	377	414	9	14	354	321
12	0	419	444	2	8	320	318	5	12	477	530	9	16	346	399
12	1	600	634	2	10	446	478	5	13	257	218	10	0	172	159
12	2	188	172	2	11	476	420	5	14	196	236	10	2	322	386
12	3	489	453	2	12	546	465	5	16	426	482	10	4	362	372
12	4	514	544	2	13	545	606	5	19	244	257	10	5	400	376
12	5	448	400	2	15	908	919	5	20	323	345	10	6	625	600
12	6	744	707	2	16	312	302	5	21	198	250	10	7	469	425
12	7	394	395	2	17	918	912	6	2	185	82	10	8	591	601
12	8	552	562	2	18	309	339	6	4	282	246	10	9	451	469
12	10	421	463	2	19	920	905	6	5	201	80	10	10	254	269
12	12	284	300	2	20	284	290	6	6	413	455	10	13	221	249
13	0	216	231	2	21	506	488	6	8	1369	1377	10	15	480	524
13	2	212	159	2	22	379	353	6	9	535	484	11	1	318	385
13	3	191	222	3	0	1523	1434	6	10	1563	1563	11	2	441	468
13	5	157	195	3	1	2022	2063	6	12	1299	1326	11	3	388	421
13	8	383	404	3	2	1086	1034	6	13	521	460	11	4	781	749
13	9	190	147	3	3	1622	1603	6	14	701	698	11	5	306	362
13	10	310	319	3	4	650	613	6	15	523	524	11	6	746	728
14	1	757	761	3	5	1391	1417	6	17	283	301	11	7	276	245
14	3	751	692	3	7	344	442	6	18	339	322	11	8	836	761
14	4	173	158	3	8	361	336	6	20	642	599	11	10	801	790
14	5	545	559	3	10	320	228	7	0	218	201	11	12	340	377
**H = -7****				3	11	1225	1218	7	1	260	245	12	0	206	131
0	0	202	242	3	13	1138	1058	7	3	325	278	12	4	499	503
0	2	255	269	3	14	342	311	7	4	742	590	12	6	535	510
0	4	724	728	3	15	232	308	7	5	220	245	12	7	202	181
0	6	679	664	3	16	593	587	7	6	1120	1173	12	8	401	389
0	8	1041	1108	3	17	298	234	7	8	1086	1137	12	9	236	263
0	10	1784	1711	3	18	222	301	7	9	216	248	12	10	553	570
0	12	1323	1407	3	19	520	486	7	10	489	521	12	12	582	609
0	14	1239	1286	3	21	351	418	7	13	277	255	12	13	161	161
0	16	999	951	4	1	283	230	7	18	175	163	13	0	180	182
0	20	565	584	4	3	279	186	7	19	145	70	13	1	688	709
0	22	644	670	4	5	373	373	8	2	234	215	13	3	396	425
1	0	822	878	4	7	929	850	8	5	657	717	13	4	365	371
1	1	1203	1227	4	8	543	453	8	7	465	455	13	5	398	423
1	2	2015	2043	4	9	920	955	8	8	399	318	13	6	427	454
1	3	1816	1748	4	10	760	792	8	10	323	326	13	7	334	363
1	4	2283	2330	4	11	983	1034	8	11	377	378	13	8	305	305
1	5	1829	1793	4	12	1012	1016	8	12	413	420	13	9	211	205
1	6	1423	1448	4	13	1456	1428	8	13	682	745	13	10	279	254
1	7	570	568	4	14	224	351	8	14	339	360	14	1	172	168
1	8	1501	1473	4	15	1275	1238	8	15	1081	1056	14	6	180	185
1	10	887	916	4	17	852	869	8	17	1238	1200	**H = -6****			
1	12	894	919	4	19	831	798	8	18	145	66	0	0	1380	1372
1	14	1169	1138	4	21	594	596	9	0	535	549	0	2	566	618
1	16	293	318	5	1	332	253	9	1	1205	1184	0	4	1959	1960
1	19	197	237	5	2	983	1141	9	2	559	579	0	6	1395	1354
1	21	257	289	5	3	725	744	9	3	1214	1180	0	8	944	935
2	0	762	713	5	4	1269	1259	9	4	751	729	0	10	1188	1073
2	1	390	306	5	5	431	460	9	5	849	868	0	12	655	746
2	2	760	718	5	6	1438	1450	9	6	652	595	0	14	637	595
2	3	460	469	5	7	323	256	9	7	372	419	0	22	181	179
2	4	1212	1182	5	8	1845	1911	9	8	281	380	1	1	190	294
2	5	1157	1191	5	9	453	511	9	10	210	193	1	2	1165	1140
2	6	228	270	5	10	1237	1234	9	11	376	332	1	3	197	155

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-6****													
1	4	317	350	4	2	1440	1323	7	8	1535	1458	11	5	225	219
1	5	1492	1444	4	3	1345	1472	7	9	379	360	11	6	326	317
1	8	1042	1169	4	4	1286	1224	7	10	1042	1025	11	7	232	284
1	9	321	316	4	5	963	921	7	11	990	942	11	8	340	315
1	10	1005	1021	4	6	1264	1374	7	12	611	614	11	9	396	395
1	11	667	685	4	7	231	246	7	13	1060	1037	11	10	438	420
1	12	667	743	4	8	1148	1103	7	14	323	305	11	12	462	413
1	13	211	236	4	9	1138	1171	7	15	1160	1133	11	13	148	199
1	14	751	790	4	10	832	831	7	17	1079	1057	11	14	163	212
1	15	272	315	4	11	1233	1210	7	18	396	374	11	15	225	221
1	17	806	801	4	13	642	610	7	19	576	586	12	2	403	368
1	18	543	585	4	14	298	320	8	0	263	290	12	4	466	429
1	19	307	347	4	15	253	157	8	1	1295	1342	12	6	653	615
1	20	837	806	4	16	251	232	8	2	237	188	12	8	769	744
1	22	747	776	4	17	247	192	8	3	1626	1673	12	10	569	628
2	0	2556	2480	4	19	413	406	8	4	394	478	12	11	155	138
2	1	2194	2181	4	20	218	170	8	5	898	924	12	12	169	175
2	2	1922	1981	4	21	368	360	8	6	379	316	12	13	148	159
2	3	2030	2064	5	1	379	460	8	7	202	211	13	2	233	193
2	4	1907	1954	5	3	182	201	8	9	378	356	13	4	455	418
2	5	1369	1355	5	4	742	871	8	12	276	298	13	6	441	457
2	6	1060	1008	5	6	1051	1071	8	13	181	139	13	8	356	348
2	7	500	416	5	7	388	375	8	14	301	312	13	10	355	351
2	8	787	827	5	8	1638	1637	8	16	200	211	13	11	147	155
2	9	370	344	5	9	817	894	8	17	200	256	14	1	480	488
2	10	567	562	5	10	1532	1613	8	19	339	319	14	2	164	183
2	11	751	800	5	11	958	896	9	0	204	93	14	3	381	392
2	12	257	248	5	12	1260	1171	9	1	477	511	14	4	352	355
2	13	406	414	5	13	756	733	9	2	220	220	14	5	311	308
2	14	316	310	5	15	574	612	9	4	275	334	14	6	283	258
2	16	222	223	5	16	446	406	9	5	464	419	14	8	126	123
2	18	275	225	5	17	507	511	9	6	569	605				
2	19	496	437	5	18	320	325	9	7	330	385	**H =	-5****		
2	21	271	283	5	19	558	535	9	8	331	339	0	0	277	313
3	0	605	606	5	20	303	327	9	11	490	480	0	2	1014	976
3	1	553	484	5	21	168	211	9	12	235	148	0	4	606	648
3	2	587	575	6	0	319	357	9	13	694	649	0	6	1399	1429
3	3	384	361	6	1	157	207	9	15	971	961	0	8	301	320
3	4	304	251	6	2	1127	953	9	17	820	818	0	12	555	452
3	5	260	366	6	3	395	359	10	0	266	285	0	14	652	638
3	6	566	537	6	4	2309	2349	10	1	801	876	0	16	421	330
3	7	282	348	6	5	292	330	10	2	558	574	0	18	1149	1123
3	8	890	905	6	6	2277	2333	10	3	640	685	0	20	1315	1242
3	9	766	728	6	7	224	188	10	4	1040	1055	1	22	772	807
3	10	477	505	6	8	1342	1381	10	5	396	418	1	0	1380	1299
3	11	1144	1153	6	9	182	26	10	6	771	784	1	1	1512	1464
3	13	1313	1351	6	10	718	713	10	7	299	250	1	2	2128	2095
3	14	178	48	6	12	321	405	10	8	478	497	1	3	1615	1633
3	15	1267	1217	6	13	457	438	10	10	395	426	1	4	1683	1681
3	17	1078	1050	6	15	308	317	10	11	318	250	1	5	413	403
3	18	212	244	6	18	257	227	10	12	420	394	1	6	1166	1270
3	19	662	657	6	20	498	513	10	15	146	221	1	8	204	303
3	20	270	270	7	0	265	88	10	16	187	220	1	10	520	551
3	21	413	402	7	2	206	200	11	1	431	420	1	12	365	459
4	0	206	246	7	3	345	386	11	2	296	246	1	13	206	187
4	1	1512	1467	7	5	491	462	11	3	438	395	1	15	246	308
				7	6	946	941	11	4	398	405	1	16	205	168
												1	22	196	173

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = -5****															
2	0	484	486	5	3	345	269	8	15	1426	1494	13	11	251	272
2	1	322	239	5	4	2535	2720	8	16	161	120	14	4	146	150
2	2	702	787	5	5	293	193	8	17	1197	1154	14	6	241	271
2	3	590	581	5	6	2442	2381	8	19	588	586	14	8	166	140
2	4	599	634	5	8	1567	1569	9	0	175	64	**H = -4****			
2	5	265	211	5	9	657	636	9	1	1241	1032	0	0	1340	1254
2	6	1003	986	5	10	825	852	9	2	298	408	0	2	2176	2138
2	7	713	651	5	11	340	376	9	3	653	665	0	4	1861	1984
2	8	322	224	5	13	436	443	9	4	583	582	0	6	1278	1206
2	9	562	653	5	14	263	288	9	6	630	517	0	8	216	166
2	10	689	732	5	15	236	165	9	7	358	349	0	10	477	423
2	11	801	736	5	18	278	261	9	8	687	660	0	12	534	414
2	12	691	661	5	19	412	383	9	9	343	332	0	14	562	560
2	13	868	869	5	20	426	421	9	10	509	501	0	16	566	560
2	14	307	182	5	21	267	233	9	12	459	406	0	18	316	254
2	15	719	787	6	0	357	403	9	16	233	257	0	20	659	646
2	16	417	411	6	1	375	439	9	17	146	183	0	22	417	428
2	17	937	886	6	2	138	104	9	18	182	167	1	0	340	324
2	18	307	374	6	3	146	232	10	0	184	100	1	1	934	941
2	19	263	276	6	4	760	697	10	1	183	109	1	2	1938	2056
2	20	555	552	6	5	413	428	10	2	182	102	1	3	561	525
2	22	627	611	6	6	1961	1920	10	4	254	237	1	4	708	672
3	0	1012	1067	6	8	2138	2176	10	5	176	195	1	6	809	779
3	1	2032	2189	6	10	1638	1683	10	8	339	337	1	7	1484	1531
3	2	554	607	6	11	412	393	10	11	414	429	1	8	808	834
3	3	1332	1377	6	12	1000	998	10	13	587	556	1	9	1230	1209
3	4	727	785	6	13	668	675	10	15	482	453	1	10	745	805
3	5	384	359	6	15	512	505	10	17	276	293	1	11	482	542
3	6	296	278	6	16	510	530	11	0	298	335	1	12	668	681
3	8	803	766	6	17	255	295	11	1	385	338	1	13	713	699
3	9	1343	1272	6	18	523	532	11	2	663	719	1	15	431	460
3	11	1235	1255	6	19	227	264	11	3	267	221	1	16	856	841
3	13	436	456	6	20	581	576	11	4	597	628	1	17	325	401
3	17	269	259	7	0	381	375	11	5	433	401	1	18	1008	998
3	19	451	418	7	1	1668	1710	11	6	625	681	1	20	946	975
3	20	223	170	7	2	1831	1934	11	7	248	226	1	21	171	143
3	21	306	347	7	3	1403	1464	11	8	704	728	1	22	642	661
4	1	373	432	7	4	1914	1983	11	10	570	552	2	0	2566	2760
4	2	253	301	7	5	813	769	11	12	173	170	2	1	3118	3252
4	4	445	428	7	6	1398	1395	11	13	262	238	2	2	1003	951
4	6	136	95	7	7	407	391	11	14	186	181	2	3	1191	1186
4	7	382	362	7	8	335	356	11	15	154	185	2	4	136	88
4	8	979	964	7	10	235	206	12	0	188	236	2	5	244	260
4	9	645	543	7	12	389	437	12	2	462	506	2	6	899	922
4	10	771	834	7	14	196	161	12	4	470	467	2	7	556	555
4	11	1356	1438	7	15	239	330	12	6	399	407	2	8	451	423
4	13	1723	1767	7	17	262	239	12	8	283	314	2	9	794	844
4	14	396	406	7	18	308	337	12	10	447	440	2	10	331	293
4	15	1123	1131	8	2	513	504	12	12	274	253	2	11	928	903
4	16	273	277	8	3	579	565	13	1	235	256	2	12	513	537
4	17	800	778	8	4	342	368	13	2	279	293	2	13	330	342
4	19	550	577	8	5	664	637	13	3	150	167	2	14	272	282
4	21	372	337	8	6	362	334	13	4	493	507	2	15	415	428
5	0	1734	1759	8	7	409	454	13	5	255	291	2	16	233	154
5	1	1289	1394	8	9	747	766	13	6	615	615	2	22	236	196
5	2	2912	2802	8	11	1058	1004	13	8	496	534	3	0	1000	993
				8	13	1192	1209	13	10	320	364	3	1	549	472

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-4****													
3	3	376	422	6	6	2209	2187	9	15	1038	1039	0	4	2684	2510
3	5	506	483	6	7	191	97	9	17	680	695	0	6	1530	1540
3	6	177	234	6	8	968	1031	9	18	166	188	0	8	2081	2041
3	8	470	469	6	9	410	393	10	0	292	330	0	10	1088	1071
3	9	284	353	6	10	822	897	10	1	236	206	0	14	928	997
3	10	746	806	6	12	600	601	10	2	784	727	0	16	1158	1140
3	11	1320	1304	6	13	463	472	10	3	245	245	0	18	1511	1438
3	12	737	738	6	14	326	365	10	4	999	962	0	20	966	968
3	13	1632	1618	6	15	197	221	10	5	279	301	0	22	425	394
3	14	726	669	6	17	257	228	10	6	899	884	1	0	1170	1180
3	15	1096	1079	6	18	230	212	10	7	356	393	1	1	1790	1781
3	17	687	698	6	19	319	334	10	8	442	433	1	2	1499	1390
3	19	331	385	6	20	331	356	10	9	310	335	1	3	378	406
3	20	175	172	7	0	568	532	10	10	263	309	1	4	1100	1194
3	21	209	159	7	1	318	344	10	11	252	193	1	5	1003	1010
4	0	2142	2122	7	2	395	423	10	14	334	306	1	6	1240	1204
4	1	627	560	7	3	160	62	10	16	343	355	1	7	1060	1002
4	2	1621	1734	7	4	805	759	10	17	146	153	1	8	588	637
4	3	734	634	7	5	393	356	11	2	180	228	1	9	445	486
4	4	1556	1533	7	6	1475	1503	11	5	232	205	1	11	871	862
4	5	554	589	7	7	731	746	11	7	287	286	1	12	280	304
4	6	726	727	7	8	1057	1081	11	8	455	490	1	13	820	789
4	7	180	154	7	9	943	897	11	9	377	397	1	14	452	392
4	8	251	269	7	10	426	357	11	10	313	341	1	15	472	418
4	9	1603	1546	7	11	1005	975	11	11	325	335	1	18	386	435
4	11	851	882	7	13	1213	1123	11	13	300	301	1	20	702	661
4	14	315	319	7	15	1243	1159	11	14	294	299	1	21	220	206
4	16	341	355	7	16	307	383	12	0	316	353	1	22	485	493
4	19	346	344	7	17	846	858	12	2	480	469	2	0	113	95
4	20	245	224	7	18	472	479	12	4	750	708	2	1	859	763
4	21	519	510	7	19	656	645	12	6	947	912	2	2	665	554
5	0	347	348	8	0	526	592	12	7	220	247	2	4	827	782
5	1	1131	1094	8	1	1627	1673	12	8	1009	1003	2	5	941	907
5	2	1130	1153	8	2	769	704	12	9	321	321	2	6	229	234
5	3	658	750	8	3	820	801	12	10	487	483	2	7	999	916
5	4	1094	972	8	4	636	627	12	11	261	236	2	8	1417	1453
5	5	161	63	8	5	168	251	13	0	275	229	2	9	1455	1416
5	6	1584	1597	8	7	379	353	13	2	341	348	2	10	1870	1761
5	7	376	346	8	8	543	597	13	4	446	427	2	11	1391	1457
5	8	1594	1589	8	9	493	521	13	6	452	445	2	12	547	550
5	9	666	678	8	10	267	198	13	8	366	367	2	13	1562	1493
5	10	1175	1141	8	11	265	273	13	9	206	180	2	14	371	299
5	11	687	730	8	13	232	253	13	10	184	195	2	15	1142	1138
5	12	348	359	8	16	163	148	13	11	384	397	2	17	500	500
5	13	565	555	8	18	183	141	14	1	493	498	2	18	202	220
5	14	249	268	9	1	284	268	14	2	269	295	2	20	500	482
5	15	497	530	9	2	318	326	14	3	291	290	2	21	191	166
5	16	345	356	9	3	257	238	14	4	351	368	2	22	246	262
5	17	349	372	9	4	338	286	14	6	310	298	3	0	1304	1406
5	18	289	258	9	6	454	470	14	7	218	215	3	1	1468	1570
5	20	390	407	9	7	341	243	14	8	217	212	3	2	1093	1083
6	0	1828	1865	9	8	317	311	14	9	266	248	3	3	592	622
6	1	221	207	9	9	641	655	15	1	127	103	3	4	288	261
6	2	3103	3232	9	11	882	898	15	4	121	153	3	5	167	155
6	3	346	346	9	12	326	273		**H =	-3****		3	6	230	209
6	4	2782	2752	9	13	957	959	0	0	186	167	3	7	1571	1518
				9	14	251	245	0	2	785	621	3	8	548	533



Table 43. Continued

**H = -3****								**H = -2****							
K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
3	9	1193	1261	6	15	284	340	10	8	366	389	1	2	136	108
3	10	449	386	6	16	586	573	10	9	685	649	1	3	172	118
3	11	1172	1080	6	17	426	389	10	10	377	379	1	4	130	126
3	12	440	390	6	18	686	713	10	11	832	805	1	5	2054	2012
3	13	251	205	6	19	384	407	10	13	640	684	1	6	1728	1736
3	14	354	373	6	20	667	669	10	15	440	428	1	7	2171	2240
3	15	253	279	7	0	1314	1274	10	16	418	426	1	8	1792	1723
3	19	257	251	7	1	1038	1067	10	17	303	352	1	9	2200	2082
3	21	280	295	7	2	1728	1761	11	0	906	889	1	10	751	733
4	0	998	1100	7	3	464	406	11	2	806	820	1	11	932	913
4	1	601	648	7	4	1569	1597	11	4	950	937	1	12	311	303
4	5	131	82	7	5	203	233	11	6	948	992	1	13	1348	1295
4	7	152	236	7	6	821	858	11	7	163	131	1	14	965	902
4	8	232	244	7	7	558	511	11	8	582	608	1	15	538	567
4	9	1041	1091	7	8	587	568	11	12	208	184	1	16	909	951
4	10	389	321	7	9	575	576	11	14	191	186	1	18	931	961
4	11	1198	1163	7	10	552	517	12	2	271	292	1	20	780	744
4	12	693	641	7	11	527	506	12	3	188	166	1	21	201	147
4	13	1135	1119	7	12	434	428	12	4	181	212	1	22	305	344
4	14	598	617	7	13	246	300	12	6	431	398	2	0	183	190
4	15	821	866	7	17	182	137	12	8	506	573	2	1	585	427
4	17	558	574	8	0	328	386	12	11	192	203	2	2	1554	1635
4	18	470	457	8	2	150	85	12	12	393	418	2	3	103	61
4	19	339	324	8	3	177	154	12	13	179	189	2	4	935	935
4	20	395	412	8	5	377	308	12	14	618	614	2	5	1573	1545
4	21	158	130	8	7	875	923	13	0	360	372	2	6	732	700
5	0	2286	2279	8	9	1061	1083	13	2	562	546	2	7	2696	2574
5	1	1892	1952	8	10	265	207	13	4	729	700	2	8	165	77
5	2	2186	2194	8	11	843	887	13	6	737	751	2	9	1427	1375
5	3	1539	1617	8	12	177	162	13	7	355	364	2	10	624	680
5	4	2103	1982	8	13	1333	1345	13	8	521	541	2	11	931	947
5	5	945	894	8	15	1314	1327	13	9	512	528	2	12	320	343
5	6	1627	1671	8	16	237	267	13	10	332	351	2	13	348	364
5	8	1548	1482	8	17	839	806	13	11	300	285	2	16	484	412
5	9	249	267	8	18	225	249	14	0	257	232	2	18	354	351
5	10	446	473	8	19	318	314	14	2	138	66	2	20	338	375
5	11	411	476	9	0	295	348	14	6	217	206	3	0	1420	1359
5	13	487	515	9	1	200	106	14	7	293	305	3	1	1486	1520
5	15	229	269	9	2	271	201	14	9	376	359	3	2	635	621
5	17	435	382	9	3	680	686	15	0	368	375	3	4	701	812
5	19	375	396	9	4	515	487	15	1	457	481	3	5	227	266
5	20	275	263	9	5	805	825	15	2	314	307	3	6	480	464
5	21	296	329	9	6	617	584	15	3	170	169	3	7	1635	1644
6	0	227	266	9	7	1062	1093	15	4	137	107	3	8	1618	1528
6	1	802	739	9	8	652	623					3	9	1952	1891
6	2	711	698	9	9	863	813	0	0	3055	3108	3	10	1123	1105
6	3	561	521	9	10	330	337	0	2	3644	4151	3	11	1635	1703
6	4	1079	1158	9	11	494	495	0	4	3952	4263	3	12	484	497
6	5	355	349	9	13	275	301	0	6	1132	1137	3	13	1648	1619
6	6	1409	1524	9	14	244	253	0	8	1305	1194	3	14	514	443
6	7	461	482	9	16	327	329	0	10	246	151	3	15	1079	1089
6	8	969	996	10	1	264	278	0	12	428	404	3	16	501	459
6	10	752	750	10	3	248	202	0	16	320	250	3	17	429	511
6	11	432	451	10	4	264	275	0	18	1111	1074	3	18	403	359
6	13	251	317	10	5	368	376	0	20	1136	1139	3	20	172	168
6	14	220	160	10	6	392	358	0	22	489	523	3	21	176	158
				10	7	397	418	1	1	108	57	4	0	586	654



Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	-2****		7	13	733	724	12	8	435	438	2	8	1149	1124
4	1	2353	2468	7	14	399	403	12	12	174	166	2	9	2044	2078
4	2	132	150	7	15	725	694	13	2	253	188	2	10	213	246
4	3	1006	1000	7	16	693	673	13	3	322	306	2	11	1828	1866
4	4	675	694	7	17	428	404	13	4	366	327	2	12	230	189
4	6	353	393	7	18	710	720	13	5	303	319	2	13	1865	1867
4	7	800	809	8	0	739	766	13	6	442	469	2	15	907	954
4	8	306	321	8	1	652	656	13	7	540	534	2	18	459	365
4	9	640	667	8	2	442	489	13	8	209	205	2	19	318	282
4	11	712	665	8	3	952	920	13	9	756	751	2	20	396	411
4	17	369	375	8	4	150	98	13	11	773	776	3	0	514	534
4	19	239	294	8	5	1003	957	13	12	163	208	3	1	2961	2948
4	20	204	254	8	7	761	796	14	0	202	163	3	2	196	181
4	21	310	292	8	9	650	637	14	1	402	422	3	3	537	558
5	0	886	827	8	11	853	860	14	4	135	117	3	4	1025	1066
5	1	593	572	8	13	447	460	14	5	410	421	3	5	1422	1411
5	2	242	161	8	16	199	169	14	6	161	147	3	6	471	431
5	3	128	61	8	17	154	127	14	7	430	460	3	7	2456	2366
5	5	290	338	9	0	401	348	14	8	154	101	3	8	913	839
5	6	1005	931	9	4	406	436	14	9	415	427	3	9	954	984
5	7	598	593	9	5	333	380	15	0	265	297	3	12	196	300
5	8	766	806	9	6	512	450	15	2	134	126	3	13	198	252
5	9	615	586	9	7	607	599	15	3	158	158	3	14	414	568
5	10	306	373	9	8	395	474					3	14	414	568
5	11	479	521	9	9	676	661		**H =	-1****		3	15	300	314
5	12	373	307	9	9	676	661	0	0	520	363	3	15	300	314
5	13	288	361	9	11	900	882	0	2	1570	1609	3	16	246	231
5	14	283	235	9	13	1164	1125	0	4	479	561	3	17	231	192
5	15	331	349	9	15	841	859	0	6	933	929	3	20	175	120
5	16	504	461	9	16	148	181	0	8	981	978	4	0	623	678
5	18	742	728	9	17	439	438	0	8	981	978	4	1	249	248
5	20	724	704	10	0	770	759	0	12	742	697	4	3	453	480
6	0	1611	1548	10	1	622	599	0	14	1897	1892	4	5	135	123
6	1	981	951	10	2	1211	1192	0	16	1578	1645	4	6	654	701
6	2	2570	2537	10	3	784	778	0	18	1002	958	4	7	1285	1313
6	3	461	358	10	4	1039	968	0	20	706	673	4	9	1440	1491
6	4	2140	2161	10	5	830	760	1	0	4898	4786	4	10	180	169
6	5	216	253	10	6	637	616	1	1	670	626	4	11	1158	1102
6	6	959	1016	10	7	1099	1011	1	2	4188	3950	4	12	447	460
6	7	505	580	10	8	299	288	1	3	536	507	4	13	480	437
6	8	1323	1310	10	9	801	825	1	4	3228	3051	4	14	512	595
6	9	313	241	10	9	801	825	1	5	1586	1570	4	15	398	398
6	10	603	664	11	1	328	356	1	6	1057	1082	4	16	685	708
6	12	266	230	11	3	354	258	1	7	1373	1399	4	18	720	687
6	14	193	240	11	4	379	364	1	8	903	852	4	20	652	634
6	15	196	224	11	5	207	169	1	9	1274	1307	4	21	274	241
6	16	329	330	11	6	684	671	1	11	1161	1196	5	0	1365	1376
6	17	466	439	11	7	225	226	1	13	256	298	5	1	1339	1304
6	20	336	338	11	8	591	559	1	14	248	287	5	2	1784	1721
7	1	487	512	11	9	468	471	1	16	922	876	5	3	641	568
7	2	202	185	11	11	273	213	1	18	821	821	5	4	2339	2319
7	3	336	381	11	12	669	639	1	20	658	706	5	5	135	109
7	4	385	372	11	13	189	151	2	0	291	270	5	6	1111	1112
7	5	218	207	11	14	756	769	2	1	82	15	5	7	628	643
7	7	369	393	12	0	929	955	2	3	497	492	5	8	494	488
7	9	531	526	12	2	969	954	2	4	412	376	5	9	694	638
7	11	572	572	12	4	1197	1227	2	5	2195	2205	5	11	468	456
				12	6	1038	1020	2	6	1544	1535	5	18	178	206
				12	7	302	272	2	7	2438	2453	5	20	335	353

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H	-	****	10	9	852	838	0	20	558	517	4	8	278	343
6	0	328	426	10	11	886	881	1	1	321	334	4	9	454	495
6	1	201	273	10	12	311	339	1	2	1281	1268	4	10	175	86
6	2	312	298	10	13	708	728	1	3	127	72	4	11	315	288
6	4	363	322	10	14	598	596	1	4	648	607	4	12	236	254
6	5	915	892	10	15	490	494	1	5	1608	1604	4	13	298	327
6	7	568	467	10	16	483	466	1	6	683	619	4	14	298	296
6	9	179	173	11	0	1303	1320	1	7	800	817	4	15	307	300
6	11	197	218	11	1	181	153	1	9	812	867	4	20	461	445
6	12	401	461	11	2	1279	1327	1	10	707	716	5	1	565	521
6	14	661	680	11	3	254	228	1	11	1460	1427	5	2	168	226
6	16	895	862	11	4	1191	1259	1	12	893	1009	5	3	366	333
6	17	277	286	11	5	564	618	1	13	1072	1082	5	4	284	196
6	18	804	798	11	6	908	860	1	14	1200	1201	5	5	1015	1054
6	20	458	495	11	7	491	530	1	15	369	332	5	6	579	575
7	0	2041	2037	11	8	186	250	1	16	897	888	5	7	802	816
7	2	1210	1179	12	3	196	199	1	17	277	252	5	8	432	407
7	3	711	661	12	4	405	443	1	18	892	932	5	9	466	466
7	4	723	764	12	5	330	295	1	20	677	741	5	10	324	281
7	5	735	692	12	6	690	708	2	0	1549	1466	5	11	352	401
7	6	658	642	12	7	366	374	2	1	856	801	5	12	744	685
7	7	916	894	12	8	324	367	2	2	1618	1517	5	13	178	119
7	8	635	664	12	9	470	444	2	3	3101	2909	5	14	743	692
7	9	453	457	12	10	424	394	2	4	767	794	5	16	705	767
7	12	356	372	12	11	488	485	2	5	1418	1455	5	17	336	346
7	13	178	117	12	12	831	839	2	6	245	247	5	18	839	843
7	14	391	326	12	13	333	334	2	7	1676	1660	5	19	220	241
7	18	215	219	13	0	567	543	2	8	951	933	5	20	477	495
8	1	354	352	13	2	664	641	2	9	1568	1489	6	0	2090	2196
8	5	657	694	13	4	629	703	2	11	399	451	6	1	447	411
8	6	166	180	13	5	579	594	2	12	713	694	6	2	1474	1472
8	7	343	296	13	6	271	270	2	14	747	650	6	3	235	42
8	9	380	409	13	7	643	621	2	15	438	423	6	4	838	795
8	10	287	379	13	9	513	469	3	1	179	122	6	6	740	777
8	11	749	755	13	11	138	119	3	2	469	407	6	7	339	389
8	13	975	958	14	0	158	186	3	3	1559	1554	6	8	158	161
8	15	549	595	14	2	209	230	3	4	336	285	6	9	310	329
8	16	351	391	14	3	204	197	3	5	1556	1485	6	10	237	208
8	18	595	573	14	4	291	294	3	7	2421	2362	6	11	434	436
9	0	262	309	14	5	532	525	3	8	272	241	6	12	679	606
9	1	400	363	14	7	625	628	3	9	1853	1901	6	14	421	437
9	2	406	484	14	9	752	756	3	10	552	527	6	17	176	121
9	3	932	1021	15	0	538	554	3	11	1732	1750	6	18	260	263
9	4	346	322	15	1	167	198	3	13	929	1028	7	1	604	531
9	5	949	1023	15	2	490	484	3	14	432	398	7	2	376	409
9	6	214	228	15	3	164	150	3	15	534	537	7	3	345	346
9	7	1080	1157	15	4	352	343	3	16	303	316	7	4	249	268
9	8	420	385	15	5	315	319	3	19	296	331	7	5	350	331
9	9	908	892		**H =	0****		3	21	437	458	7	7	193	198
9	10	395	400	0	2	4900	6128	4	0	1812	1804	7	9	285	192
9	11	382	345	0	4	1987	2015	4	1	1457	1458	7	12	423	388
9	15	186	170	0	6	950	829	4	2	291	298	7	13	180	151
10	0	321	321	0	8	220	177	4	3	367	424	7	14	746	730
10	4	721	758	0	10	361	284	4	4	1352	1346	7	15	206	117
10	6	686	640	0	14	470	539	4	5	949	968	7	16	806	813
10	7	335	393	0	16	1263	1166	4	6	1421	1359	7	17	153	99
10	8	257	240	0	18	703	758	4	7	1375	1375	7	18	565	564

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	0****													
7	19	387	377	13	2	317	271	2	11	1560	1589	6	0	337	426
8	0	528	511	13	3	295	333	2	12	608	574	6	2	229	341
8	1	679	613	13	4	506	451	2	13	1036	1032	6	3	361	369
8	2	581	605	13	5	717	732	2	14	487	488	6	4	266	301
8	3	1293	1331	13	6	295	234	2	15	586	570	6	5	720	691
8	4	237	211	13	7	806	809	2	16	395	408	6	6	229	160
8	5	1138	1182	13	9	925	918	2	18	700	694	6	8	233	236
8	7	619	644	13	10	243	242	2	19	265	243	6	9	393	332
8	8	278	290	13	11	614	608	2	20	538	523	6	10	762	784
8	9	525	568	14	0	247	216	2	21	338	345	6	11	315	274
8	10	276	275	14	1	233	253	3	0	519	534	6	12	1208	1245
8	11	245	273	14	2	249	268	3	3	701	749	6	13	179	98
8	15	246	185	14	3	595	593	3	4	849	876	6	14	1315	1296
8	16	190	216	14	4	319	333	3	5	1906	1876	6	16	910	877
8	18	312	306	14	5	807	775	3	6	1327	1290	6	18	498	513
9	1	290	295	14	6	239	256	3	7	1103	1147	6	19	182	146
9	5	463	468	14	7	746	697	3	8	1017	915	7	0	2045	2037
9	7	746	756	14	9	364	395	3	9	1028	954	7	1	447	416
9	8	367	306	15	3	157	173	3	10	309	336	7	2	1425	1426
9	9	942	910	15	4	188	212	3	11	170	194	7	3	1259	1301
9	10	216	211	15	5	320	340	3	12	818	754	7	4	548	465
9	11	976	1019		**H =	1****		3	13	516	551	7	5	1624	1571
9	12	351	350	0	0	486	363	3	14	421	358	7	6	253	212
9	13	874	876	0	2	834	753	3	15	462	443	7	7	942	944
9	14	263	261	0	4	927	878	3	16	270	200	7	10	605	559
9	15	516	477	0	10	626	568	4	0	619	678	7	11	430	442
10	0	1147	1056	0	12	827	897	4	1	242	274	7	12	661	671
10	1	284	193	0	14	1398	1384	4	2	619	614	7	13	283	289
10	2	952	997	0	16	1355	1206	4	4	1458	1384	7	16	324	332
10	3	617	580	0	18	842	881	4	5	1184	1137	7	18	433	395
10	4	425	434	0	20	775	811	4	6	2272	2255	7	19	259	251
10	5	1002	979	1	0	5446	4786	4	7	1290	1354	8	1	731	828
10	6	548	510	1	1	1050	969	4	8	1131	1080	8	2	417	419
10	7	989	959	1	2	2298	2254	4	9	1487	1481	8	3	702	664
10	8	533	536	1	3	1101	1054	4	10	553	549	8	4	526	636
10	9	309	304	1	4	1445	1463	4	11	658	708	8	5	663	696
10	10	197	225	1	5	1420	1444	4	12	656	634	8	6	587	582
10	16	248	236	1	6	281	249	4	14	767	772	8	7	293	283
11	1	425	368	1	7	1180	1219	4	16	638	708	8	8	658	653
11	2	703	650	1	8	447	428	4	17	461	468	8	9	651	638
11	4	1026	932	1	9	1529	1486	4	18	594	555	8	11	848	893
11	5	253	301	1	11	408	420	4	19	553	613	8	13	501	496
11	6	983	974	1	14	282	276	4	20	296	249	8	14	328	333
11	9	233	207	1	15	251	233	5	0	1368	1376	8	16	379	341
11	10	354	423	1	16	309	282	5	1	852	878	8	17	338	318
11	11	252	218	1	18	295	232	5	2	1727	1799	8	18	218	222
11	12	841	791	1	20	336	260	5	3	1067	1066	9	0	295	309
11	14	735	759	2	0	302	270	5	4	1066	1025	9	1	201	206
12	0	1307	1373	2	1	409	370	5	5	344	316	9	2	226	247
12	2	1237	1260	2	2	674	659	5	7	545	561	9	3	702	681
12	4	937	959	2	3	2958	2788	5	8	549	564	9	4	411	396
12	5	197	202	2	5	1140	1122	5	9	674	671	9	5	908	891
12	6	363	323	2	6	685	667	5	11	571	601	9	6	200	168
12	7	188	165	2	7	1872	1886	5	12	414	335	9	7	648	636
12	9	228	278	2	8	509	477	5	13	313	368	9	9	400	374
13	1	252	273	2	9	2238	2146	5	18	400	392	9	10	222	188
				2	10	1062	1004	5	20	428	407	9	13	283	273

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	1****		0	2	3733	3756	4	3	1195	1238	7	16	546	548
10	0	262	321	0	4	330	315	4	4	636	595	7	17	295	274
10	2	710	729	0	8	940	903	4	5	1433	1489	7	18	248	242
10	4	394	395	0	10	496	519	4	6	769	783	8	0	778	766
10	5	177	89	0	12	842	904	4	7	1332	1289	8	1	1305	1346
10	6	234	274	0	14	468	364	4	9	630	624	8	2	788	839
10	7	823	848	0	16	329	322	4	11	282	357	8	3	1341	1347
10	8	179	199	0	18	347	324	4	13	535	524	8	4	970	1018
10	9	733	786	1	1	144	86	4	15	338	304	8	5	1428	1416
10	10	343	310	1	3	531	497	4	18	341	330	8	6	478	481
10	11	724	746	1	4	367	373	4	19	186	165	8	7	1095	1091
10	12	626	658	1	5	329	339	4	20	277	280	8	8	203	210
10	13	651	616	1	6	634	649	5	0	891	827	8	9	383	370
10	14	667	652	1	7	358	330	5	1	460	501	8	13	498	473
10	15	452	428	1	8	1004	934	5	2	320	328	8	14	232	212
10	16	377	356	1	9	613	668	5	3	605	635	8	16	361	355
11	0	1331	1320	1	10	565	596	5	4	1313	1391	8	17	272	281
11	2	1218	1181	1	11	993	1020	5	5	362	341	9	0	390	348
11	3	354	298	1	12	998	1007	5	6	149	134	9	1	507	541
11	4	748	687	1	13	426	486	5	7	313	333	9	3	856	829
11	5	576	606	1	14	1191	1168	5	8	800	806	9	4	582	517
11	6	386	392	1	16	1048	1032	5	10	1500	1521	9	5	760	745
11	7	383	361	1	18	907	865	5	12	1443	1451	9	6	643	677
11	8	328	374	1	20	614	576	5	13	433	420	9	7	1047	1009
12	1	224	187	2	0	166	190	5	14	1525	1398	9	8	426	455
12	2	364	406	2	1	1610	1609	5	15	486	474	9	9	1070	1049
12	4	489	602	2	2	159	91	5	16	1058	1038	9	10	340	350
12	5	403	471	2	3	201	199	5	17	322	357	9	11	989	1001
12	6	296	327	2	4	877	860	5	18	541	587	9	12	508	496
12	7	403	384	2	5	1470	1378	5	19	428	401	9	13	482	525
12	9	508	501	2	6	712	725	6	0	1619	1548	9	14	367	317
12	10	478	465	2	7	986	1061	6	1	720	705	9	15	203	181
12	11	240	261	2	8	563	571	6	2	1000	1116	9	16	191	154
12	12	498	500	2	9	895	939	6	3	502	500	10	0	777	759
12	13	205	180	2	11	325	440	6	5	918	883	10	1	340	279
13	0	591	543	2	13	386	385	6	6	151	175	10	2	245	197
13	1	188	215	2	16	219	112	6	7	183	236	10	3	339	349
13	2	402	349	2	18	284	215	6	8	639	642	10	5	874	878
13	3	527	583	2	20	186	199	6	9	518	499	10	7	485	457
13	5	853	855	3	0	1416	1359	6	10	995	987	10	8	528	515
13	7	803	817	3	1	893	836	6	11	396	353	10	9	189	171
13	9	372	362	3	2	1355	1384	6	12	673	683	10	15	168	151
13	11	150	127	3	3	1477	1531	6	16	603	559	11	2	677	692
14	0	215	186	3	4	916	995	6	18	493	504	11	4	695	690
14	1	188	168	3	5	2264	2268	6	19	190	201	11	5	177	65
14	2	449	454	3	6	1580	1568	7	1	1392	1398	11	6	225	217
14	3	340	363	3	7	2452	2448	7	3	653	635	11	10	532	510
14	4	258	272	3	8	837	842	7	4	436	436	11	11	247	241
14	5	498	514	3	9	1911	1937	7	5	582	608	11	12	533	539
14	7	577	596	3	11	966	982	7	6	265	299	11	13	150	184
15	0	541	554	3	13	601	584	7	7	532	557	11	14	576	558
15	1	425	461	3	17	519	568	7	9	226	249	12	0	944	955
15	2	545	532	3	18	206	208	7	10	469	494	12	2	670	707
15	3	503	493	3	19	689	699	7	11	340	342	12	4	359	357
15	4	467	510	4	0	582	654	7	12	923	939	12	5	298	309
	**H =	2****		4	1	1514	1490	7	13	346	320	12	7	253	238
0	0	3073	3108	4	2	1546	1501	7	14	904	908	12	10	137	68

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 2****															
12	11	248	221	2	7	1256	1285	6	0	279	266	10	7	768	775
12	12	137	125	2	8	746	790	6	1	795	784	10	9	552	575
13	2	188	222	2	9	1289	1311	6	3	263	328	10	10	845	810
13	4	146	147	2	10	578	525	6	4	728	758	10	11	376	368
13	5	354	326	2	11	850	837	6	5	968	886	10	12	854	835
13	7	376	398	2	12	388	380	6	6	421	400	10	13	311	265
13	9	260	243	2	14	835	812	6	7	391	347	10	14	707	718
13	10	249	261	2	15	377	407	6	8	1328	1342	11	0	896	889
14	0	187	163	2	16	921	943	6	9	295	228	11	1	220	181
14	1	659	643	2	17	359	372	6	10	1811	1779	11	2	615	598
14	2	354	384	2	18	549	545	6	12	1563	1553	11	3	577	575
14	3	751	693	2	19	464	410	6	13	272	314	11	4	277	280
14	4	225	227	3	0	1319	1406	6	14	1308	1316	11	5	399	362
14	5	744	742	3	1	2841	2830	6	16	697	721	11	6	227	143
14	6	170	189	3	2	853	899	6	18	413	404	11	11	305	281
14	7	649	643	3	3	1943	1943	7	0	1289	1274	11	14	225	212
14	8	173	230	3	5	1799	1731	7	1	1630	1572	12	0	204	201
15	0	296	297	3	6	658	624	7	2	1045	1004	12	3	198	107
15	1	126	123	3	7	1303	1225	7	3	1807	1730	12	4	288	284
15	2	190	200	3	8	452	417	7	4	328	288	12	7	227	226
15	3	327	326	3	9	1020	997	7	5	1892	1878	12	8	249	281
15	4	133	121	3	10	206	133	7	7	1144	1070	12	10	354	353
**H = 3****				3	11	711	678	7	8	889	896	12	12	416	426
0	0	184	167	3	12	440	415	7	9	307	369	13	0	391	372
0	2	2644	2509	3	13	366	403	7	10	514	515	13	1	349	368
0	4	2032	1998	3	19	276	291	7	13	373	353	13	3	598	586
0	6	606	634	4	0	1010	1100	7	14	404	402	13	5	494	498
0	8	485	456	4	1	539	506	7	16	485	531	13	6	230	229
0	10	233	130	4	2	1532	1490	7	17	336	316	13	7	288	301
0	12	863	770	4	3	411	437	7	18	286	318	13	9	205	187
0	14	657	727	4	4	1493	1390	8	0	352	386	13	10	125	127
0	16	856	860	4	5	1929	1869	8	1	1192	1204	14	0	256	232
0	18	626	588	4	6	635	629	8	2	348	317	14	3	177	195
0	20	449	464	4	7	1784	1812	8	3	1197	1229	14	7	176	201
1	0	1204	1180	4	8	661	646	8	4	613	633	15	0	385	375
1	1	186	130	4	9	1078	1066	8	5	1042	1107	15	1	565	565
1	2	1840	1805	4	10	1388	1453	8	6	457	453	15	2	221	209
1	3	1377	1343	4	11	560	515	8	7	947	938	15	3	504	533
1	4	259	257	4	12	977	1031	8	9	666	680	**H = 4****			
1	5	1032	1014	4	14	805	819	8	10	220	232	0	0	1368	1254
1	6	391	390	4	15	539	536	8	11	885	878	0	2	578	600
1	7	1400	1343	4	16	586	593	8	12	381	376	0	4	361	312
1	8	857	854	4	17	743	751	8	14	230	217	0	6	293	244
1	10	1101	1116	4	19	803	783	8	15	221	219	0	8	1256	1282
1	11	305	343	5	0	2298	2279	8	17	221	218	0	10	1440	1488
1	12	852	857	5	1	1146	1072	9	0	318	348	0	12	399	353
1	13	390	452	5	2	1257	1242	9	1	642	629	0	14	310	285
1	14	335	307	5	3	596	604	9	2	531	426	0	16	570	528
1	16	404	385	5	4	436	397	9	3	1009	1008	0	18	362	363
1	18	504	463	5	5	636	616	9	4	382	382	1	0	337	324
1	20	164	195	5	6	241	209	9	5	1351	1346	1	1	731	684
2	2	1023	1018	5	7	595	665	9	7	748	720	1	2	818	718
2	3	907	866	5	8	333	355	9	9	265	270	1	3	198	235
2	4	190	226	5	9	388	427	9	10	280	249	1	4	611	620
2	5	959	966	5	10	280	211	10	3	309	343	1	5	953	880
2	6	886	864	5	16	557	558	10	4	239	227	1	6	687	719
				5	18	512	502	10	5	580	640	1	9	388	370

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
1	10	768	703	5	6	985	968	9	9	659	630	1	11	652	624
1	12	588	618	5	7	866	905	9	10	476	472	1	13	227	179
1	13	419	390	5	8	1561	1522	9	11	277	271	1	14	431	416
1	14	478	491	5	9	1043	1025	9	12	589	589	1	15	254	249
1	16	721	644	5	10	1930	1910	9	13	150	79	1	16	402	441
1	18	270	299	5	12	1623	1592	9	14	483	482	1	18	428	390
1	19	220	201	5	14	1311	1329	9	15	249	280	2	0	492	486
2	0	2670	2760	5	15	617	623	9	16	218	214	2	1	269	196
2	1	1946	1885	5	16	880	869	10	0	313	330	2	2	691	688
2	2	1935	1974	5	17	310	360	10	1	379	384	2	3	552	545
2	3	1264	1203	5	18	249	296	10	2	219	203	2	4	378	341
2	4	214	253	6	0	1856	1865	10	3	835	893	2	5	666	683
2	5	1845	1837	6	1	706	803	10	4	288	299	2	6	767	773
2	6	1021	983	6	2	509	494	10	5	886	907	2	7	1006	1005
2	7	1353	1339	6	3	1368	1374	10	6	206	172	2	8	850	779
2	8	234	308	6	4	718	750	10	7	331	303	2	9	674	667
2	10	623	616	6	5	901	946	10	9	195	123	2	10	481	444
2	12	568	485	6	6	891	832	11	3	232	205	2	12	523	547
2	15	345	313	6	7	349	365	11	5	358	319	2	13	462	468
2	16	434	479	6	8	640	626	11	8	511	468	2	14	466	505
2	18	435	459	6	9	207	222	11	10	661	658	2	15	843	898
2	19	287	261	6	10	401	436	11	12	630	683	2	16	522	474
3	0	997	993	6	14	482	486	12	0	343	353	2	17	745	768
3	1	310	265	6	16	565	576	12	2	182	245	2	19	502	500
3	2	713	706	6	17	201	171	12	5	199	111	3	0	1035	1067
3	3	1692	1648	6	18	390	380	12	8	177	137	3	1	3014	2904
3	4	140	172	7	0	546	532	12	11	187	211	3	2	1142	1177
3	5	1494	1493	7	1	750	765	13	0	269	229	3	3	2735	2680
3	6	446	478	7	3	999	1044	13	3	138	127	3	4	309	368
3	7	1292	1381	7	5	776	828	13	8	194	213	3	5	1304	1333
3	8	355	353	7	6	174	183	14	1	551	601	3	6	209	138
3	9	1347	1319	7	7	634	592	14	3	515	563	3	7	647	708
3	10	546	489	7	8	909	890	14	4	208	203	3	9	445	399
3	11	660	638	7	9	470	521	14	5	399	363	3	10	641	663
3	14	375	359	7	10	1106	1109	14	7	323	299	3	11	446	472
3	15	706	775	7	11	476	516	15	1	246	227	3	16	616	556
3	16	438	388	7	12	1023	1026	0	**H =	5***	3	17	283	302	
3	17	1011	1006	7	14	523	549	0	0	290	313	3	18	215	247
3	19	695	718	7	15	177	162	0	2	197	135	3	19	393	376
4	0	2156	2122	7	16	303	307	0	4	320	335	4	0	126	163
4	1	2971	2986	8	0	541	592	0	8	826	828	4	1	814	699
4	2	955	955	8	1	1839	1802	0	10	1138	1087	4	2	258	222
4	3	2534	2406	8	2	539	562	0	12	661	718	4	3	1327	1383
4	4	391	413	8	3	1994	1978	0	14	361	318	4	5	1729	1771
4	5	2165	2131	8	5	1874	1894	0	16	290	317	4	6	864	959
4	7	597	607	8	7	1183	1167	0	18	156	203	4	7	1543	1413
4	8	263	147	8	8	233	205	1	0	1423	1299	4	8	1404	1448
4	9	369	313	8	9	453	429	1	1	485	391	4	9	978	973
4	10	348	309	8	10	202	169	1	2	906	869	4	10	1080	1068
4	11	191	105	8	11	257	242	1	3	803	784	4	11	543	543
4	17	239	245	8	13	227	154	1	4	203	171	4	12	764	764
4	19	330	375	8	15	272	287	1	5	369	372	4	14	577	577
5	0	358	348	9	1	962	900	1	6	998	980	4	15	677	677
5	1	462	362	9	3	1211	1176	1	7	352	306	4	16	438	413
5	2	696	833	9	5	1059	1043	1	8	1396	1367	4	17	742	730
5	3	329	436	9	6	250	233	1	9	599	639	5	0	1762	1759
				9	7	647	718	1	10	948	908	5	1	1516	1570

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	5****		10	3	580	636	2	1	2182	2199	6	6	585	654
5	2	610	611	10	5	648	611	2	2	1461	1345	6	7	354	296
5	3	146	180	10	8	521	500	2	3	1222	1140	6	8	214	147
5	4	831	841	10	9	223	179	2	5	304	367	6	9	243	208
5	5	461	518	10	10	857	893	2	6	364	362	6	10	335	339
5	6	672	594	10	11	286	258	2	8	582	522	6	11	206	141
5	9	298	293	10	12	837	833	2	9	214	247	6	13	243	244
5	13	276	236	10	13	261	286	2	10	400	393	6	15	246	239
5	16	273	220	10	14	521	542	2	14	370	449	7	2	425	378
6	0	346	403	11	0	345	335	2	15	234	257	7	3	714	783
6	1	292	163	11	1	547	448	2	16	639	614	7	4	208	243
6	2	296	339	11	3	397	404	2	17	222	261	7	5	531	515
6	3	1157	1129	11	6	241	246	2	18	255	235	7	6	212	212
6	4	320	337	11	8	254	293	3	0	599	606	7	7	438	430
6	5	712	756	11	10	210	173	3	1	1489	1523	7	8	979	1035
6	6	691	712	11	12	154	193	3	2	1237	1212	7	9	371	407
6	8	1418	1421	12	0	183	236	3	3	1508	1562	7	10	909	898
6	9	425	418	12	2	223	171	3	5	1170	1163	7	11	222	121
6	10	1458	1450	12	6	161	176	3	6	327	336	7	12	502	476
6	12	1205	1158	12	7	171	150	3	7	676	640	7	14	411	374
6	14	752	754	12	8	485	495	3	9	392	461	7	15	170	199
6	16	597	561	12	10	506	531	3	12	218	152	7	16	304	312
7	0	367	375	13	1	410	462	3	13	518	493	8	0	175	290
7	1	2025	1998	13	3	405	412	3	15	1098	1081	8	1	1210	1279
7	3	2063	2095	13	4	176	213	3	17	921	986	8	2	590	577
7	4	300	212	13	5	150	167	4	0	215	246	8	3	1410	1388
7	5	1354	1335	13	6	206	208	4	1	2206	2142	8	4	610	524
7	6	672	740	14	1	145	136	4	3	1985	2026	8	5	1209	1149
7	7	778	818	14	3	285	353	4	4	835	824	8	6	402	416
7	8	608	657	14	5	303	334	4	5	527	508	8	7	794	859
7	9	415	396					4	6	301	391	8	8	372	414
7	12	310	344	0	0	1446	1372	4	7	251	244	8	10	290	260
7	14	184	182	0	4	387	372	4	11	256	258	8	11	218	264
7	17	276	277	0	6	507	608	4	12	547	510	8	14	227	227
8	1	903	980	0	8	1146	1087	4	16	165	123	9	0	198	93
8	3	1167	1093	0	10	641	628	4	17	187	198	9	1	853	931
8	4	415	450	0	12	492	481	4	18	152	127	9	3	645	612
8	5	1009	987	0	14	629	680	5	2	403	436	9	4	853	820
8	6	620	635	0	16	325	412	5	4	529	462	9	5	402	463
8	7	504	528	0	18	205	178	5	5	813	876	9	6	399	371
8	8	680	651	1	1	371	354	5	6	963	1003	9	8	300	301
8	9	470	461	1	2	162	49	5	7	1236	1261	9	10	383	405
8	10	388	364	1	3	339	299	5	8	1405	1326	9	11	466	480
8	12	245	239	1	4	287	209	5	9	875	917	9	12	390	358
8	13	284	282	1	5	317	306	5	10	944	960	9	13	480	485
8	15	304	304	1	6	1096	1069	5	11	549	551	9	14	214	220
9	1	1612	1589	1	7	419	428	5	12	1263	1217	10	0	275	285
9	2	212	195	1	8	1548	1598	5	14	919	938	10	1	1078	1091
9	3	1537	1517	1	10	1360	1422	5	15	253	245	10	3	982	996
9	4	629	657	1	11	571	586	5	16	593	542	10	5	212	235
9	5	1504	1508	1	12	981	947	5	17	250	223	10	6	532	500
9	7	877	832	1	13	504	567	6	0	285	357	10	8	431	447
9	8	348	315	1	14	276	290	6	1	966	914	10	10	180	206
9	14	181	188	1	15	526	488	6	2	594	642	10	13	141	61
9	15	216	222	1	17	392	365	6	3	1021	1018	11	2	288	207
10	1	211	223	1	19	283	309	6	4	307	351	11	4	346	263
10	2	183	226	2	0	2580	2480	6	5	482	410	11	6	514	526



Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 6****												**H = 8****			
11	7	278	290	2	17	839	841	7	5	482	521	0	0	972	997
11	8	831	828	3	0	1540	1434	7	6	644	671	0	2	1355	1332
11	9	222	218	3	1	1985	2029	7	8	462	392	0	4	1211	1211
11	10	788	753	3	2	847	852	7	13	249	241	0	6	1621	1565
11	12	712	702	3	3	1819	1856	8	0	174	121	0	8	824	876
12	1	378	343	3	4	711	726	8	1	265	181	0	10	288	331
12	2	440	431	3	5	719	659	8	2	560	625	0	14	298	245
12	3	318	318	3	14	258	243	8	3	488	605	0	16	180	170
12	4	667	674	3	15	179	119	8	4	552	601	0	2	632	604
12	6	493	432	3	16	366	368	8	6	573	520	1	3	358	384
12	8	181	168	3	17	363	363	8	7	271	286	1	4	1458	1452
12	10	157	148	4	1	436	492	8	8	443	446	1	5	1088	1052
13	1	230	187	4	2	745	731	8	10	308	297	1	6	1796	1905
13	3	411	399	4	3	1444	1355	8	11	452	446	1	7	430	531
13	5	241	240	4	4	1162	1176	8	13	400	423	1	8	1964	2032
13	8	331	328	4	5	905	937	8	15	452	461	1	10	1384	1429
14	1	641	641	4	6	1003	1026	9	0	538	549	1	11	500	506
14	3	534	560	4	7	650	645	9	1	1293	1264	1	12	486	507
**H = 7****				4	8	754	759	9	2	445	395	1	13	566	585
0	0	225	242	4	9	595	591	9	3	1217	1146	1	14	276	283
0	2	479	553	4	10	469	438	9	4	168	66	1	15	527	534
0	4	1050	1021	4	11	418	420	9	5	733	659	1	17	570	554
0	6	1821	1712	4	12	729	665	9	6	221	206	2	0	546	476
0	8	2362	2471	4	13	410	364	9	7	371	343	2	1	1910	1880
0	10	2095	2194	4	14	363	349	9	11	164	120	2	2	600	515
0	12	1003	943	4	15	619	649	9	12	194	228	2	3	1869	1864
0	14	219	264	4	16	156	140	10	1	387	365	2	4	422	357
1	0	921	878	4	17	504	515	10	2	168	102	2	5	618	549
1	1	281	300	5	1	392	428	10	3	466	440	2	6	246	228
1	2	194	182	5	2	655	620	10	4	190	228	2	7	235	177
1	3	364	395	5	3	516	487	10	6	608	614	2	8	603	596
1	4	384	483	5	4	795	693	10	7	300	336	2	9	350	324
1	6	919	896	5	6	402	417	10	8	768	765	2	10	308	259
1	7	481	497	5	7	516	527	10	9	530	473	2	13	223	247
1	8	1050	1040	5	8	412	417	10	10	728	698	2	15	498	490
1	9	254	295	5	10	817	746	10	11	550	505	2	16	193	162
1	10	342	424	5	11	319	284	10	12	481	493	2	17	432	436
1	12	246	257	5	12	426	439	11	0	197	229	3	0	575	626
1	13	336	337	5	13	274	263	11	2	702	725	3	1	994	986
1	14	519	451	5	15	161	174	11	4	861	799	3	3	662	666
1	15	386	361	5	17	134	60	11	6	559	549	3	4	327	321
1	16	406	376	6	1	422	437	11	8	341	348	3	7	249	125
1	17	198	193	6	3	536	487	11	10	250	212	3	10	224	270
2	0	711	713	6	4	268	265	12	3	277	304	3	11	453	496
2	1	707	701	6	6	411	319	12	6	505	508	3	12	452	448
2	2	172	155	6	7	346	460	12	8	628	654	3	13	1093	1105
2	3	583	650	6	8	481	459	12	9	137	125	3	14	382	382
2	4	1096	1041	6	9	237	208	13	0	209	182	3	15	922	949
2	5	1122	1032	6	10	884	939	13	1	702	662	3	16	152	185
2	6	1043	1066	6	11	214	183	13	2	293	273	3	17	567	589
2	8	882	892	6	12	901	868	13	3	399	381	4	0	757	865
2	10	778	807	6	14	683	658	13	4	302	312	4	1	1323	1332
2	11	698	681	6	16	390	381	13	6	305	346	4	2	727	733
2	12	454	423	7	0	265	201	13	7	124	44	4	3	971	883
2	13	974	947	7	1	786	803	14	1	353	406	4	4	977	941
2	15	1033	1028	7	2	436	522	14	2	155	98	4	5	353	372
				7	3	634	584	14	3	391	388				



Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	8****		9	9	529	551	2	5	573	568	8	2	259	263
4	6	733	712	9	11	640	639	2	6	935	889	8	3	454	432
4	7	210	66	9	13	652	624	2	8	628	610	8	4	407	364
4	8	662	696	10	0	238	155	2	9	493	535	8	5	390	369
4	10	595	638	10	1	870	868	2	11	704	695	8	6	521	506
4	13	254	266	10	2	667	624	2	12	192	158	8	8	430	401
4	14	167	132	10	3	586	592	2	13	980	979	8	9	419	456
4	15	295	302	10	4	705	737	2	14	212	205	8	10	332	252
4	17	253	270	10	5	244	202	2	15	770	787	8	11	658	631
5	1	185	142	10	6	395	388	2	16	215	180	8	12	190	149
5	2	242	254	10	8	389	340	3	0	297	265	8	13	426	455
5	3	274	311	10	11	254	246	3	1	1622	1618	9	0	226	178
5	4	485	461	11	2	228	265	3	2	262	218	9	1	1247	1209
5	5	629	553	11	3	205	212	3	3	1126	1109	9	2	309	299
5	6	317	337	11	4	559	566	3	4	514	514	9	3	987	947
5	7	542	511	11	5	158	138	3	9	218	294	9	5	324	313
5	8	441	446	11	6	853	845	3	11	343	299	9	11	154	134
5	9	299	176	11	8	867	801	3	13	258	251	9	12	166	172
5	10	777	754	11	10	788	767	3	14	178	166	10	1	701	654
5	12	723	738	12	0	438	444	3	15	381	380	10	3	572	513
5	14	378	354	12	1	570	625	4	2	300	253	10	4	581	597
6	0	205	117	12	2	819	812	4	4	447	443	10	6	603	589
6	1	284	192	12	3	294	272	4	5	251	222	10	8	590	599
6	2	264	268	12	4	654	650	4	6	457	573	10	9	195	252
6	6	461	437	12	6	368	360	4	8	442	445	10	10	260	277
6	8	783	719	12	8	164	138	4	9	208	192	10	11	460	450
6	9	245	179	13	0	237	231	4	10	694	683	11	0	795	767
6	11	297	277	13	1	375	377	4	11	611	568	11	2	1078	1078
6	13	336	334	13	3	275	282	4	12	424	428	11	4	912	885
6	15	144	123	13	5	161	139	4	13	623	647	11	6	513	414
7	1	335	316	14	1	627	619	4	14	168	133	11	8	240	256
7	3	239	216		**H =	9****		4	15	514	513	11	9	193	201
7	6	510	560	0	2	997	1069	4	16	241	210	12	0	187	186
7	8	846	814	0	4	1552	1603	5	0	851	773	12	2	212	256
7	10	735	665	0	6	2499	2604	5	1	374	393	12	4	544	519
7	11	328	260	0	8	2387	2299	5	2	699	797	12	6	646	648
7	12	357	377	0	10	1405	1414	5	3	367	319	12	7	215	220
7	13	341	310	0	12	532	570	5	4	509	499	13	0	244	244
7	14	247	277	0	14	475	405	5	6	805	722	13	1	638	601
7	15	221	221	1	0	531	587	5	7	292	233	13	2	346	333
8	1	718	727	1	1	1571	1569	5	8	858	830	13	3	372	361
8	2	260	271	1	2	1739	1741	5	10	383	381	13	4	326	325
8	3	390	519	1	3	1023	1026	5	11	260	285		**H =	10****	
8	4	296	312	1	4	1561	1582	5	13	389	436	0	0	1182	1129
8	5	598	630	1	6	990	1042	5	14	306	286	0	2	1387	1399
8	6	527	506	1	7	453	430	5	15	220	232	0	4	1292	1327
8	8	615	607	1	8	602	619	6	1	382	455	0	6	1117	1081
8	9	255	245	1	10	353	332	6	4	326	268	0	8	408	354
8	10	465	426	1	11	447	447	6	6	436	484	0	10	359	336
8	11	235	222	1	12	258	216	6	8	809	741	0	12	532	561
8	12	180	142	1	13	380	400	6	10	721	677	0	14	139	79
8	14	147	155	1	15	305	292	6	12	421	428	1	0	360	322
9	2	287	374	1	17	351	344	7	4	903	825	1	1	480	482
9	3	310	347	2	1	922	912	7	5	271	270	1	2	1130	1164
9	5	263	191	2	2	810	900	7	6	687	622	1	3	916	956
9	6	160	58	2	3	383	417	7	14	178	150	1	4	1244	1277
9	8	431	395	2	4	1224	1211	8	1	388	297	1	5	652	634

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
		**H = 10****													
1	6	1614	1642	5	14	236	237	12	3	234	195	4	12	194	140
1	8	1046	1022	6	0	274	330	12	4	320	327	4	13	735	719
1	9	288	250	6	1	206	96	12	6	155	185	5	0	1275	1233
1	10	393	370	6	2	777	762	13	1	270	293	5	2	1144	1067
1	11	389	389	6	3	286	213	13	2	175	186	5	3	261	261
1	12	232	215	6	4	1039	949			**H = 11****		5	4	626	658
1	13	416	389	6	5	366	299	0	2	748	776	5	5	477	453
1	15	506	490	6	6	576	651	0	4	1264	1261	5	6	395	392
2	0	1707	1717	6	8	273	273	0	6	1659	1613	5	8	271	271
2	1	1551	1585	6	10	282	273	0	8	774	776	5	10	213	229
2	2	1142	1224	6	11	175	161	0	10	301	305	5	11	169	134
2	3	1208	1263	6	12	266	258	0	12	474	461	5	12	415	401
2	4	513	471	7	1	695	660	1	0	976	929	5	13	146	141
2	6	441	407	7	3	486	513	1	1	1396	1325	6	0	302	216
2	7	226	276	7	4	783	746	1	2	855	901	6	1	391	346
2	8	413	395	7	6	1161	1168	1	3	580	572	6	2	712	716
2	10	386	377	7	7	216	251	1	4	832	817	6	4	1211	1233
2	13	269	289	7	8	832	791	1	5	184	76	6	6	1329	1335
2	15	187	242	7	9	437	473	1	6	502	491	6	8	871	926
2	16	154	152	7	10	377	393	1	8	442	427	6	9	237	228
3	0	609	578	7	11	544	482	1	10	395	396	6	10	333	321
3	2	384	409	7	12	241	228	1	11	205	230	6	11	250	244
3	5	303	384	7	13	443	461	2	0	498	471	6	13	172	145
3	6	380	413	8	1	950	904	2	1	530	590	7	0	438	482
3	7	267	255	8	2	303	266	2	2	613	547	7	1	468	428
3	8	556	542	8	3	771	681	2	3	222	254	7	2	898	835
3	9	443	444	8	4	589	606	2	4	293	358	7	3	247	265
3	10	499	519	8	6	318	329	2	6	191	99	7	4	771	815
3	11	973	981	8	12	206	164	2	7	299	229	7	1	608	604
3	12	338	362	8	0	184	244	2	9	437	407	8	2	201	100
3	13	973	959	9	1	475	408	2	11	556	578	8	3	319	356
3	14	306	333	9	3	475	490	2	12	249	183	8	6	346	371
3	15	642	647	9	4	314	260	2	13	603	626	8	7	535	544
4	0	963	954	9	5	254	251	2	14	345	356	8	8	298	297
4	1	688	705	9	9	488	424	2	15	685	669	8	9	726	751
4	2	791	768	9	9	197	163	3	0	523	514	8	10	192	202
4	3	249	209	9	10	519	542	3	1	484	420	8	11	695	758
4	4	628	611	9	11	620	623	3	3	453	427	8	11	695	758
4	5	330	335	10	0	728	756	3	3	426	352	9	0	251	226
4	6	658	720	10	1	717	796	3	4	426	352	9	1	828	793
4	7	289	333	10	2	272	247	3	5	250	237	9	2	221	261
4	9	357	349	10	3	628	590	3	7	444	484	9	3	295	326
4	12	333	349	10	4	181	180	3	9	567	504	9	10	157	109
4	13	445	450	10	5	300	284	3	10	256	242	9	10	157	109
4	14	369	332	10	6	222	190	3	11	192	202	10	0	265	299
4	15	308	306	10	9	229	271	3	13	245	253	10	1	391	431
5	2	341	328	11	0	358	431	4	0	338	345	10	2	270	323
5	4	573	589	11	1	527	478	4	1	337	310	10	3	213	211
5	5	306	208	11	2	191	160	4	2	322	285	10	4	316	373
5	6	671	721	11	3	689	635	4	3	578	568	10	5	195	200
5	7	344	354	11	4	251	241	4	4	508	446	10	6	278	257
5	8	801	779	11	5	540	554	4	5	694	682	10	8	130	138
5	9	285	300	11	6	278	299	4	6	694	637	11	0	777	721
5	10	605	663	11	7	542	556	4	7	508	433	11	2	640	584
5	12	188	175	11	8	607	604	4	8	645	601	11	4	353	339
5	13	243	270	11	8	542	556	4	9	658	657	11	5	236	242
				12	0	225	258	4	10	311	352	11	6	251	292
				12	1	562	611	4	11	936	942	12	0	354	376
				12	2			4	11			12	2	446	460

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
		**H = 11****		5	6	807	842	2	5	349	316	9	2	371	391
12	4	306	381	5	7	381	388	2	6	432	391	9	3	171	179
		**H = 12****		5	8	677	753	2	7	396	442	9	4	405	381
0	0	267	219	5	9	405	403	2	8	404	432	9	5	221	220
0	2	503	456	5	10	248	208	2	9	541	550	9	7	121	145
0	4	708	735	5	11	309	315	2	10	167	191	10	4	155	153
0	6	590	533	5	12	310	300	2	11	508	512	10	5	139	143
0	8	406	405	6	0	1344	1255	2	12	185	177	11	0	475	487
0	10	293	246	6	2	1073	1058	2	13	477	475	11	2	389	379
0	12	156	121	6	4	957	966	3	0	484	436	11	3	157	195
0	14	155	173	6	6	346	337	3	3	486	532			**H = 14****	
1	1	583	581	6	10	136	75	3	4	363	329	0	0	591	678
1	2	422	404	7	1	248	338	3	5	689	655	0	2	681	679
1	3	242	156	7	2	375	406	3	7	729	727	0	4	463	447
1	4	698	738	7	4	1091	1088	3	9	275	307	0	6	375	398
1	6	530	512	7	5	435	418	3	10	195	206	0	8	275	238
1	7	379	387	7	6	950	975	3	11	167	187	0	12	144	161
1	8	392	426	7	7	757	780	3	12	230	239	1	2	613	606
1	9	248	264	7	8	421	425	4	0	411	448	1	3	280	294
1	11	213	231	7	9	924	911	4	2	239	176	1	4	870	825
1	13	329	334	7	11	801	780	4	3	333	351	1	5	556	562
1	14	353	352	8	1	689	685	4	4	265	245	1	6	628	638
2	0	732	750	8	2	254	284	4	5	270	291	1	7	417	435
2	1	583	540	8	6	155	68	4	6	219	191	1	8	340	324
2	4	221	246	8	7	188	166	4	7	723	662	1	9	384	343
2	5	182	205	8	9	130	31	4	9	807	786	1	10	141	98
2	6	388	341	9	0	366	317	4	11	735	767	1	11	177	189
2	7	407	407	9	1	369	319	4	12	120	116	1	12	401	382
2	8	348	321	9	5	196	154	5	0	1354	1394	2	2	206	180
3	0	214	233	9	7	442	441	5	1	200	200	2	3	600	630
3	2	193	137	9	9	532	525	5	2	977	1004	2	4	446	420
3	3	485	545	10	0	618	624	5	4	886	840	2	5	636	636
3	4	410	402	10	1	317	265	5	5	412	422	2	6	204	226
3	5	290	280	10	2	433	435	5	6	371	411	2	7	281	294
3	6	236	263	10	3	206	191	5	10	158	186	2	10	244	237
3	7	255	262	10	4	258	303	6	0	576	650	3	3	186	210
3	9	663	652	10	6	170	128	6	2	1013	959	3	4	183	180
3	11	965	943	11	0	372	358	6	4	1288	1337	3	5	248	295
3	12	173	147	11	1	231	261	6	6	961	989	3	6	497	485
3	13	715	711	11	2	233	214	6	7	242	244	3	7	701	666
4	0	1048	1009	11	4	142	168	6	8	493	469	3	8	403	392
4	1	266	228	12	0	346	355	6	9	414	394	3	9	778	787
4	2	975	981	12	2	303	313	6	11	376	359	3	10	269	240
4	3	465	491			**H = 13****		7	0	887	893	3	11	544	574
4	4	363	376	0	2	440	366	7	1	306	306	4	0	743	740
4	5	445	450	0	4	839	825	7	2	849	916	4	1	190	218
4	6	194	136	0	6	668	663	7	3	236	150	4	2	592	599
4	7	427	459	0	8	389	369	7	4	510	540	4	3	344	304
4	8	207	117	0	12	356	301	7	6	194	191	4	4	321	303
4	9	208	214	1	0	279	238	7	8	208	197	4	5	733	744
4	10	338	305	1	2	225	166	8	1	324	354	4	7	423	415
4	12	161	153	1	4	368	410	8	2	213	116	4	11	234	252
4	13	202	198	1	6	485	500	8	4	147	116	5	0	760	691
5	0	624	634	1	8	225	249	8	5	608	597	5	2	887	789
5	2	615	676	1	12	192	228	8	7	878	909	5	4	689	708
5	4	893	917	2	3	205	188	8	9	782	794	5	5	296	293
5	5	269	271	2	4	228	175	9	0	332	330	5	6	618	571

Table 43. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 14****															
5	7	318	355	3	7	214	287	3	4	520	513	4	4	143	165
5	8	229	218	3	8	193	176	3	5	592	598	4	5	409	416
5	9	230	266	4	0	306	315	3	6	498	471	5	0	290	321
5	10	176	147	4	1	258	206	3	7	619	656	5	1	216	214
6	0	1502	1569	4	2	236	199	3	8	160	174	5	2	332	323
6	2	1097	1066	4	3	226	173	4	2	207	184	5	3	286	279
6	4	649	646	4	5	333	370	4	3	195	203	5	4	203	211
6	6	310	351	4	7	608	595	4	4	179	142	5	5	142	143
6	8	148	158	4	8	156	139	4	5	348	368	6	0	217	200
7	0	485	391	5	0	938	935	4	7	201	192	6	1	272	263
7	2	713	690	5	2	633	623	4	8	116	83	6	2	181	141
7	3	256	261	5	3	219	154	5	0	327	336	6	3	352	354
7	4	535	548	5	4	503	485	5	1	222	285	6	4	104	31
7	5	557	578	5	5	176	248	5	2	358	366	7	0	290	317
7	7	768	753	5	5	176	248	5	3	311	303	7	2	151	139
8	0	253	211	5	6	261	257	5	4	269	241	7	3	128	125
8	3	368	334	6	0	651	635	5	5	224	240	**H = 18****			
8	4	260	225	6	2	617	668	5	6	201	224	0	0	532	544
8	5	293	347	6	4	420	420	5	7	176	137	0	2	182	146
8	6	176	73	6	6	291	268	6	0	838	838	1	0	221	207
9	2	231	195	6	7	207	218	6	2	480	485	1	1	436	462
9	3	228	237	7	0	852	853	6	4	288	265	1	2	265	241
9	4	307	306	7	2	373	386	6	6	149	158	1	3	488	501
9	5	484	495	7	6	140	141	7	0	209	232	1	5	411	400
9	6	217	229	8	3	321	345	7	2	247	299	2	1	557	598
10	0	598	616	8	4	133	149	7	5	231	222	2	3	571	585
10	2	487	505	8	5	527	560	8	0	151	57	2	4	140	121
10	3	149	144	9	0	486	479	8	1	356	350	2	5	384	388
11	0	123	136	9	1	462	471	8	2	175	165	3	0	261	235
**H = 15****				9	2	435	437	8	3	260	267	3	1	408	424
0	0	879	835	9	3	427	434	9	0	138	113	3	2	156	138
0	2	1215	1193	10	0	143	157	9	1	139	106	3	3	582	573
0	4	934	947	10	1	124	182	**H = 17****				3	5	687	687
0	6	275	324	**H = 16****				0	0	397	401	4	0	294	319
0	8	130	87	0	0	1338	1278	0	2	505	542	4	1	343	359
0	10	372	397	0	2	494	539	0	4	261	250	4	2	270	276
1	0	1083	1046	1	0	538	510	0	6	176	172	4	3	399	391
1	1	315	304	1	1	598	566	1	0	579	623	5	0	187	147
1	2	523	506	1	2	730	762	1	1	588	511	5	1	316	332
1	3	638	598	1	3	693	705	1	2	325	318	5	2	256	240
1	5	238	246	1	4	663	645	1	3	417	424	5	3	344	328
1	9	192	171	1	5	629	633	1	5	374	354	6	0	355	342
2	1	451	394	1	6	262	273	1	7	171	201	**H = 19****			
2	2	423	448	1	7	317	304	2	1	616	630	0	0	148	106
2	3	523	537	1	8	144	174	2	2	416	372	1	0	136	166
2	4	647	693	1	9	341	349	2	3	631	653	1	1	410	406
2	5	883	889	2	0	244	213	2	4	475	472	1	2	113	73
2	6	799	783	2	1	627	626	2	5	700	699	1	3	304	315
2	7	644	598	2	2	258	234	2	6	131	193	2	1	589	565
2	8	321	313	2	3	599	641	2	7	644	615	2	3	635	625
2	9	508	569	2	4	209	200	3	1	267	275	3	0	300	272
3	0	214	216	2	5	338	342	3	3	282	306	3	1	530	524
3	3	535	489	2	8	116	59	3	5	298	315	3	2	241	246
3	4	268	238	3	1	356	368	4	1	224	233	4	0	310	310
3	5	622	679	3	2	291	275	4	2	154	171	4	1	314	333
				3	3	413	456	4	3	393	373	5	0	424	406

Table 44. 10\*(Fobs vs. Fcal) For [Rh2Br2(mu-CO)(DPM)2].

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
**L = -21****				9	1	368	366	9	1	582	558	-9	0	420	472
1	0	772	794	10	1	542	569	12	1	405	397	-7	0	817	833
3	0	388	381	12	1	405	325	13	1	430	524	-5	0	1235	1273
5	0	637	698	13	1	337	326	-7	2	265	265	-3	0	921	937
7	0	406	304	-4	2	559	572	-6	2	258	209	-1	0	782	838
4	1	288	315	-3	2	331	357	-5	2	430	421	1	0	514	418
5	1	503	491	2	2	286	326	-3	2	536	531	3	0	1003	978
**L = -20****				4	2	296	241	-2	2	509	496	5	0	416	459
-2	0	234	197	7	2	451	431	1	2	683	695	7	0	504	593
0	0	258	284	10	2	649	662	2	2	333	297	11	0	471	460
2	0	272	270	12	2	477	452	3	2	699	721	13	0	396	369
4	0	422	409	13	2	409	346	6	2	1020	990	15	0	579	612
-3	1	344	317	-5	3	587	571	7	2	701	693	-10	1	254	173
-1	1	424	438	-3	3	246	183	9	2	461	492	-8	1	398	398
0	1	409	411	-1	3	342	307	14	2	370	337	-6	1	417	394
1	1	338	433	1	3	360	394	-4	3	471	475	-4	1	838	833
2	1	396	385	2	3	490	552	-2	3	319	341	-1	1	346	365
3	1	558	588	5	3	513	496	1	3	325	283	0	1	781	813
4	1	330	312	7	3	329	327	2	3	392	316	1	1	445	429
7	1	573	520	9	3	516	513	3	3	438	454	2	1	723	775
10	1	538	518	10	3	937	845	4	3	559	545	4	1	657	610
0	2	261	220	11	3	631	555	6	3	363	361	6	1	652	540
2	2	265	278	12	3	323	349	7	3	414	437	8	1	667	667
3	2	410	431	-2	4	626	644	8	3	506	478	9	1	660	700
6	2	750	701	-1	4	408	295	9	3	460	441	11	1	458	499
7	2	662	541	0	4	284	302	11	3	872	818	14	1	600	624
8	2	363	384	1	4	527	459	14	3	347	388	15	1	586	600
9	2	1033	968	2	4	279	295	-6	4	453	504	-7	2	415	353
0	3	261	245	3	4	990	990	-4	4	250	206	-2	2	284	248
1	3	359	337	4	4	319	247	-3	4	251	188	5	2	496	379
4	3	745	702	5	4	293	371	4	4	553	449	7	2	862	829
7	3	495	453	6	4	762	738	7	4	586	516	8	2	1141	1143
8	3	654	601	9	4	578	613	10	4	819	778	10	2	1119	1165
1	4	330	242	11	4	578	531	12	4	517	501	12	2	340	364
2	4	449	378	-1	5	715	679	13	4	399	393	13	2	397	381
5	4	339	318	2	5	520	442	-4	5	330	351	15	2	461	515
6	4	289	235	4	5	305	296	-3	5	640	589	16	2	1096	1120
**L = -19****				7	5	579	619	-1	5	759	755	-9	3	437	458
-5	0	923	956	**L = -18****				2	5	715	745	-8	3	245	266
-3	0	854	918	-8	0	332	329	3	5	624	616	-7	3	341	372
-1	0	464	454	-6	0	316	254	4	5	352	286	-6	3	436	470
1	0	1033	1078	0	0	298	300	5	5	690	757	-3	3	445	390
3	0	574	596	2	0	308	335	7	5	526	518	-2	3	320	120
5	0	934	933	8	0	643	658	11	5	675	675	-1	3	473	458
7	0	404	374	10	0	330	274	-2	6	1010	951	2	3	466	546
9	0	690	692	12	0	685	700	0	6	943	911	5	3	816	676
11	0	408	502	14	0	611	654	1	6	305	280	6	3	606	618
13	0	271	359	-8	1	320	288	3	6	267	200	9	3	903	782
-5	1	593	590	-6	1	606	603	4	6	536	541	11	3	663	670
-4	1	651	692	-4	1	557	629	6	6	621	606	14	3	868	846
-3	1	376	381	-1	1	280	228	8	6	621	597	15	3	608	624
-2	1	252	209	0	1	524	534	9	6	389	337	-8	4	425	416
0	1	648	654	2	1	512	469	2	7	227	277	-7	4	761	793
1	1	340	197	4	1	521	562	3	7	486	456	-5	4	885	927
2	1	548	575	5	1	411	374	4	7	331	283	-2	4	866	890
4	1	585	601	6	1	395	327	5	7	878	892	1	4	761	708
8	1	1206	1100	7	1	446	345	**L = -17****				3	4	835	817

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
**L = -17****				-3	1	629	701	13	4	866	841	-8	1	339	312
6	4	570	546	0	1	361	424	14	4	377	367	-7	1	339	281
8	4	308	286	1	1	865	921	15	4	680	652	-5	1	945	973
9	4	388	330	2	1	344	366	16	4	428	408	-4	1	312	226
13	4	290	308	3	1	632	609	-9	5	447	385	-3	1	378	359
-7	5	258	250	5	1	534	427	-6	5	464	464	-2	1	564	491
-6	5	508	436	7	1	705	676	-5	5	356	353	-1	1	882	861
-3	5	555	626	9	1	1023	1093	-4	5	398	328	1	1	677	662
-2	5	414	366	13	1	491	458	-3	5	661	660	3	1	715	663
-1	5	543	484	15	1	521	571	-2	5	813	840	4	1	582	544
0	5	289	271	16	1	399	421	-1	5	481	454	5	1	859	900
1	5	405	451	-11	2	613	596	0	5	338	145	6	1	1053	955
2	5	294	291	-10	2	571	536	2	5	523	468	10	1	520	554
3	5	330	396	-7	2	578	544	3	5	801	786	11	1	480	449
4	5	304	379	-5	2	581	683	4	5	486	409	14	1	340	340
5	5	531	545	-4	2	326	321	6	5	570	640	15	1	314	342
6	5	632	598	-3	2	480	472	9	5	309	380	16	1	853	880
7	5	371	314	-2	2	752	799	11	5	558	568	18	1	647	684
8	5	393	294	-1	2	319	382	13	5	315	258	-11	2	245	222
9	5	383	271	0	2	300	173	14	5	841	763	-6	2	450	503
11	5	408	345	1	2	836	837	15	5	471	449	-4	2	698	754
2	5	464	471	3	2	544	596	-7	6	294	341	-1	2	728	710
3	6	603	580	8	2	703	657	-4	6	488	439	0	2	994	946
4	6	639	660	9	2	405	491	-2	6	558	583	2	2	907	905
2	6	290	311	11	2	372	432	0	6	514	540	4	2	1115	1147
3	6	276	270	15	2	658	685	4	6	323	209	5	2	637	643
5	6	732	703	17	2	1083	1131	7	6	272	305	7	2	1178	1102
6	6	531	469	-9	3	435	413	10	6	376	404	8	2	1251	1217
7	6	752	732	-8	3	245	288	-4	7	355	357	9	2	434	538
9	6	658	683	-6	3	580	581	-1	7	525	493	10	2	781	800
10	6	462	467	-5	3	453	473	0	7	323	399	12	2	503	545
12	6	301	230	-4	3	451	481	1	7	274	289	14	2	367	351
-3	7	396	375	-3	3	435	360	3	7	526	509	15	2	389	341
-1	7	562	540	-2	3	312	312	4	7	456	469	16	2	297	290
1	7	287	271	0	3	706	735	5	7	401	447	-12	3	480	463
4	7	318	315	2	3	388	427	6	7	348	361	-11	3	278	279
6	7	580	597	3	3	726	636	8	7	610	630	-10	3	488	457
8	7	477	488	6	3	546	484	12	7	735	758	-8	3	294	319
**L = -16****				9	3	899	930	-2	8	206	93	-6	3	356	248
-8	0	503	534	10	3	676	618	1	8	551	565	-4	3	272	176
-6	0	697	644	11	3	900	881	3	8	452	453	-3	3	633	621
-4	0	934	1000	12	3	340	345	5	8	891	926	1	3	767	821
-2	0	284	256	14	3	331	319	7	8	675	704	2	3	413	343
0	0	1253	1333	16	3	451	482	9	8	317	286	3	3	372	463
2	0	1314	1268	17	3	700	679	**L = -15****				6	3	1200	1155
4	0	926	946	-10	4	511	464	-13	0	817	846	7	3	598	517
8	0	1041	1058	-4	4	276	327	-11	0	620	5	8	3	343	247
10	0	433	345	-3	4	399	431	-9	0	537	583	10	3	490	515
12	0	833	963	-1	4	640	604	-7	0	273	211	13	3	411	409
14	0	306	230	2	4	1079	975	-5	0	710	699	14	3	951	1025
16	0	977	1091	3	4	389	323	1	0	593	606	15	3	674	708
-11	1	303	259	4	4	1083	1062	3	0	290	280	16	3	735	796
-8	1	716	719	5	4	801	722	7	0	599	530	18	3	525	573
-7	1	446	442	7	4	842	833	13	0	724	788	-10	4	827	849
-6	1	698	709	8	4	434	544	17	0	1026	1111	-7	4	572	592
-5	1	313	237	9	4	497	391	-12	1	571	571	-5	4	404	456
-4	1	665	706	10	4	851	766	-9	1	285	189	-4	4	438	437

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-15****		6	7	875	840	18	1	572	594	7	4	376	361
-2	4	489	472	8	7	415	358	19	1	325	313	8	4	453	431
-1	4	302	319	9	7	359	285	-13	2	786	781	10	4	796	733
0	4	362	387	12	7	599	609	-11	2	476	452	11	4	405	343
1	4	608	525	13	7	839	842	-10	2	329	376	12	4	387	388
2	4	414	475	-4	8	468	460	-9	2	260	260	18	4	464	443
3	4	813	756	-2	8	482	467	-7	2	308	302	-11	5	378	337
5	4	644	676	0	8	525	443	-6	2	632	633	-10	5	682	699
9	4	467	449	2	8	236	260	-5	2	518	549	-8	5	444	524
10	4	494	497	5	8	249	201	-2	2	323	320	-7	5	537	487
11	4	788	773	6	8	391	348	-1	2	325	287	-5	5	562	511
12	4	292	312	0	9	465	472	0	2	620	614	-4	5	369	406
14	4	937	919	2	9	245	204	2	2	372	338	-2	5	1368	1325
15	4	294	361	3	9	223	146	6	2	1527	1468	0	5	631	637
16	4	517	545	4	9	683	665	7	2	1067	1054	1	5	820	774
17	4	380	333	5	9	522	519	8	2	833	857	3	5	322	264
-9	5	626	627	6	9	790	765	9	2	1333	1366	5	5	774	816
-8	5	446	482	7	9	405	506	10	2	673	734	6	5	487	463
-7	5	597	603		**L =	-14****		11	2	538	603	9	5	803	793
-6	5	376	398	-12	0	610	623	14	2	613	644	10	5	320	303
-4	5	528	485	-8	0	957	936	15	2	1238	1350	13	5	951	931
-3	5	370	376	-6	0	986	1065	17	2	1379	1441	14	5	606	527
-2	5	820	808	-4	0	1250	1295	18	2	506	543	17	5	265	215
0	5	574	565	0	0	1895	1884	19	2	473	509	-10	6	606	568
1	5	978	978	2	0	1163	1209	-13	3	502	495	-8	6	420	388
3	5	1269	1266	4	0	1474	1431	-11	3	472	455	-3	6	288	311
4	5	1028	1004	6	0	416	482	-10	3	544	533	-1	6	535	557
6	5	863	838	8	0	725	714	-7	3	533	492	4	6	813	738
10	5	440	381	10	0	451	555	-6	3	476	510	6	6	589	617
11	5	341	324	12	0	416	482	-4	3	286	273	11	6	411	464
12	5	803	771	14	0	326	407	-3	3	320	261	12	6	673	663
15	5	643	673	16	0	540	553	-2	3	854	922	14	6	846	815
-9	6	380	391	18	0	694	627	-1	3	368	398	16	6	544	499
-7	6	476	428	-14	1	584	597	0	3	523	495	-8	7	606	565
-6	6	426	402	-12	1	1132	1138	1	3	838	821	-6	7	291	185
-5	6	457	425	-11	1	839	849	3	3	356	345	-4	7	629	656
-3	6	1316	1227	-8	1	441	446	4	3	803	731	-2	7	746	731
-1	6	1254	1282	-7	1	563	566	6	3	1006	1004	0	7	477	481
1	6	373	316	-6	1	329	382	8	3	974	922	7	7	489	443
2	6	876	864	-5	1	409	420	9	3	1114	1160	8	7	702	646
3	6	710	750	-3	1	832	800	10	3	713	759	11	7	592	545
5	6	898	913	-2	1	446	409	11	3	726	671	13	7	847	814
7	6	892	873	-1	1	984	939	13	3	746	782	-7	8	488	469
8	6	338	382	0	1	543	558	15	3	722	753	-6	8	262	176
9	6	523	479	1	1	1310	1331	16	3	876	904	-5	8	385	377
10	6	637	601	2	1	772	776	17	3	275	281	-3	8	345	366
11	6	522	438	3	1	1101	1074	18	3	367	378	-1	8	581	628
13	6	725	723	4	1	402	442	-11	4	436	468	1	8	460	473
15	6	260	283	5	1	404	307	-9	4	692	697	3	8	760	763
-7	7	287	273	7	1	1482	1521	-8	4	391	317	5	8	712	708
-5	7	495	482	8	1	590	659	-6	4	977	980	7	8	460	491
-4	7	310	356	9	1	630	745	-3	4	871	848	11	8	613	605
-2	7	307	295	10	1	434	561	-2	4	360	197	-4	9	393	382
-1	7	287	308	12	1	566	568	-1	4	612	680	0	9	709	696
0	7	503	573	15	1	503	519	0	4	381	315	2	9	253	193
4	7	853	821	16	1	761	775	2	4	1316	1283	4	9	464	494
5	7	770	748	17	1	420	448	5	4	1109	1024	5	9	407	402



H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
**L = -14****				2	2	404	516	12	4	584	588	7	7	390	444
6	9	243	251	3	2	321	328	14	4	1210	1241	8	7	386	339
7	9	475	491	4	2	388	367	15	4	315	268	11	7	517	546
10	9	218	259	5	2	906	810	17	4	281	274	13	7	923	911
4	10	385	371	8	2	492	479	18	4	588	559	14	7	341	368
**L = -13****				9	2	526	554	19	4	300	371	15	7	388	393
-15	0	472	479	11	2	782	862	-11	5	245	187	-8	8	438	441
-13	0	781	823	14	2	301	257	-10	5	258	294	-6	8	312	291
-5	0	730	772	16	2	871	961	-9	5	316	298	-3	8	257	203
-3	0	394	321	17	2	350	310	-8	5	650	611	4	8	884	898
-1	0	1161	1190	18	2	993	991	-7	5	501	551	6	8	829	804
1	0	1641	1593	19	2	376	369	-5	5	555	586	7	8	254	229
3	0	1289	1272	20	2	290	270	-4	5	906	959	8	8	483	409
5	0	685	607	-13	3	516	528	-3	5	587	621	9	8	313	274
7	0	765	789	-12	3	398	407	-2	5	460	505	10	8	597	640
9	0	748	732	-11	3	561	602	-1	5	774	715	12	8	1639	1619
11	0	1119	1238	-10	3	682	653	1	5	866	860	14	8	838	851
13	0	977	1071	-7	3	745	759	2	5	627	600	-5	9	268	280
15	0	976	1038	-5	3	343	339	3	5	1056	1015	-4	9	421	356
17	0	807	799	-4	3	427	490	4	5	754	725	-2	9	445	426
-15	1	230	215	-3	3	711	802	5	5	884	918	0	9	553	567
-14	1	234	214	-2	3	798	863	7	5	711	647	1	9	569	602
-13	1	839	786	-1	3	294	243	10	5	1114	1069	2	9	275	259
-11	1	416	428	1	3	528	518	12	5	376	303	4	9	592	584
-9	1	466	436	2	3	561	542	14	5	306	372	5	9	736	714
-7	1	953	963	3	3	365	331	15	5	783	757	6	9	273	228
-6	1	374	349	4	3	400	383	16	5	300	333	7	9	358	314
-5	1	1651	1640	5	3	409	390	17	5	276	185	8	9	354	326
-4	1	444	427	6	3	869	791	18	5	327	363	9	9	476	541
-3	1	476	456	7	3	948	901	-11	6	728	708	11	9	622	672
-2	1	596	606	8	3	694	716	-10	6	430	384	-3	10	693	700
-1	1	793	837	9	3	438	427	-9	6	870	865	-1	10	666	642
0	1	1244	1333	10	3	1057	1086	-6	6	662	612	1	10	476	474
2	1	888	922	11	3	707	711	-5	6	741	768	2	10	557	531
3	1	351	477	12	3	567	601	-4	6	420	298	3	10	541	552
4	1	511	483	13	3	635	618	-3	6	1469	1427	4	10	207	163
5	1	775	703	14	3	443	471	-1	6	1427	1378	6	10	234	119
6	1	375	223	16	3	382	394	1	6	500	473	**L = -12****			
8	1	1242	1385	17	3	874	887	2	6	1076	1006	-16	0	310	281
10	1	413	504	18	3	818	832	3	6	794	760	-14	0	696	734
12	1	489	477	19	3	293	256	5	6	331	405	-12	0	1080	1063
16	1	1236	1252	-14	4	240	232	7	6	387	438	-10	0	669	666
17	1	425	390	-12	4	333	370	10	6	310	375	-8	0	1069	1062
19	1	477	478	-11	4	337	313	12	6	318	299	-6	0	865	884
20	1	304	295	-8	4	364	324	15	6	375	290	-4	0	1553	1545
-14	2	701	710	-6	4	451	401	16	6	305	261	-2	0	613	534
-12	2	810	786	-5	4	482	501	-10	7	290	322	0	0	857	809
-11	2	740	730	-2	4	400	449	-9	7	708	691	4	0	628	666
-9	2	421	436	1	4	688	658	-8	7	588	586	6	0	618	642
-8	2	487	480	2	4	548	578	-4	7	452	475	10	0	805	817
-7	2	414	394	3	4	1862	1854	-3	7	393	418	12	0	409	431
-6	2	797	800	4	4	364	385	-2	7	762	718	14	0	694	701
-4	2	1187	1220	5	4	1032	989	0	7	714	722	16	0	434	461
-3	2	948	976	6	4	762	725	1	7	573	572	18	0	868	927
-2	2	373	446	9	4	1246	1171	4	7	495	590	20	0	286	293
-1	2	709	726	10	4	498	511	5	7	794	772	-15	1	272	256
0	2	1043	1143	11	4	1238	1220	6	7	472	544	-14	1	229	290



Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L = -12****			7	3	416	355	18	5	425	409	0	9	480	516
-13	1	486	465	8	3	1617	1581	-8	6	300	339	2	9	235	251
-12	1	397	438	10	3	466	489	-5	6	678	683	3	9	372	396
-11	1	484	541	12	3	462	426	-4	6	955	928	5	9	885	951
-9	1	331	309	13	3	958	1030	-2	6	1305	1308	6	9	723	725
-6	1	799	859	14	3	870	893	0	6	819	832	7	9	837	907
-5	1	779	776	15	3	1190	1173	1	6	344	417	8	9	349	363
-3	1	291	315	16	3	465	547	4	6	1449	1390	11	9	687	692
-2	1	576	579	19	3	384	409	5	6	1007	1001	12	9	580	550
-1	1	1149	1165	20	3	410	401	6	6	1553	1484	13	9	546	500
0	1	1196	1210	-15	4	504	529	8	6	643	654	-5	10	616	636
2	1	1481	1430	-14	4	963	953	9	6	686	655	-4	10	738	748
3	1	600	611	-12	4	474	500	11	6	528	544	-2	10	887	890
4	1	744	715	-11	4	926	887	12	6	817	802	-1	10	310	297
6	1	462	439	-9	4	645	701	13	6	888	798	0	10	768	749
7	1	1059	1192	-8	4	611	612	14	6	538	522	1	10	438	454
8	1	734	771	-7	4	461	411	16	6	318	290	3	10	209	148
9	1	455	499	-6	4	977	1029	17	6	273	240	4	10	887	911
10	1	309	401	-3	4	1051	991	-12	7	706	666	5	10	410	353
12	1	600	627	-1	4	323	340	-11	7	563	525	6	10	901	917
13	1	312	329	0	4	309	311	-10	7	938	927	8	10	768	789
16	1	689	758	2	4	513	485	-9	7	515	530	9	10	205	204
17	1	1061	1134	3	4	365	354	-8	7	623	621	10	10	216	197
18	1	330	290	4	4	755	720	-6	7	543	586	2	11	573	576
-14	2	357	360	5	4	424	493	-4	7	836	787	3	11	493	519
-12	2	365	342	6	4	638	579	-2	7	581	540				
-9	2	554	553	7	4	387	382	-1	7	732	727	**L = -11****			
-7	2	286	341	9	4	318	50	0	7	491	470	-13	0	375	373
-6	2	725	732	11	4	548	528	2	7	743	711	-7	0	1475	1381
-3	2	330	309	12	4	516	576	3	7	542	611	-5	0	2052	2051
-2	2	835	817	13	4	374	403	5	7	1069	1037	-3	0	427	451
-1	2	438	368	14	4	593	619	6	7	352	327	-1	0	1871	1957
0	2	384	348	15	4	846	836	7	7	758	784	1	0	2016	2105
1	2	858	875	16	4	407	406	9	7	422	345	3	0	1257	1295
3	2	880	915	19	4	748	737	11	7	833	803	5	0	448	525
6	2	1675	1735	-13	5	338	274	12	7	742	758	7	0	1910	1903
7	2	1561	1572	-12	5	231	196	13	7	753	715	9	0	1063	1146
8	2	289	221	-10	5	1011	998	14	7	627	603	11	0	725	731
9	2	1484	1574	-8	5	538	501	15	7	480	428	13	0	561	535
10	2	525	558	-7	5	1050	1056	15	7	480	428	15	0	1030	1014
11	2	585	637	-6	5	355	361	-9	8	952	931	19	0	565	582
14	2	868	890	-4	5	283	263	-7	8	446	388	21	0	585	550
15	2	852	902	-3	5	1468	1456	-5	8	602	600	-15	1	557	534
16	2	289	292	-2	5	650	668	-3	8	426	443	-13	1	1137	1090
17	2	473	511	-1	5	741	697	-1	8	834	951	-11	1	334	285
-15	3	593	585	0	5	481	469	3	8	618	625	-10	1	782	821
-13	3	873	898	1	5	510	538	4	8	393	386	-9	1	617	603
-12	3	503	536	2	5	1211	1128	9	8	486	478	-8	1	924	958
-10	3	642	655	3	5	845	740	11	8	662	679	-7	1	1158	1168
-5	3	385	352	4	5	336	395	13	8	1396	1353	-6	1	693	636
-4	3	283	311	5	5	1475	1466	14	8	271	266	-5	1	1010	1068
-2	3	869	921	6	5	426	422	15	8	348	334	-4	1	1215	1185
0	3	558	548	7	5	511	413	-8	9	779	757	-3	1	385	338
1	3	484	504	10	5	1102	933	-7	9	233	245	-2	1	223	69
2	3	578	495	11	5	508	447	-6	9	366	366	0	1	1585	1672
4	3	859	805	13	5	765	723	-4	9	554	576	1	1	599	652
6	3	535	544	16	5	326	385	-3	9	341	387	2	1	860	878
								-1	9	379	427	3	1	356	303

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
		**L = -11****													
4	1	844	776	-2	3	466	568	5	5	922	917	1	8	504	470
5	1	843	833	-1	3	417	444	6	5	331	375	2	8	312	275
6	1	1277	1334	2	3	1068	1074	7	5	1267	1207	4	8	1283	1270
7	1	836	935	4	3	612	601	8	5	318	138	6	8	603	615
8	1	2294	2451	5	3	1423	1447	10	5	918	899	8	8	784	781
9	1	639	671	6	3	466	406	11	5	670	596	10	8	448	492
10	1	376	399	8	3	445	446	14	5	620	601	12	8	1027	1013
11	1	556	580	9	3	1248	1333	15	5	357	370	-8	9	462	449
12	1	458	475	10	3	1498	1499	19	5	327	291	-7	9	240	200
14	1	354	344	11	3	748	794	-14	6	355	362	-5	9	377	336
15	1	516	530	12	3	817	836	-13	6	302	318	-3	9	401	489
16	1	471	544	13	3	495	487	-12	6	349	273	-1	9	594	618
17	1	799	814	14	3	428	425	-11	6	706	724	0	9	344	321
18	1	327	417	15	3	694	765	-10	6	419	468	1	9	557	536
19	1	589	573	17	3	1111	1132	-9	6	698	717	3	9	612	640
20	1	375	368	18	3	536	521	-8	6	612	630	6	9	488	452
21	1	250	214	20	3	394	395	-7	6	340	285	9	9	455	521
-16	2	603	598	-15	4	235	211	-6	6	809	748	10	9	332	370
-14	2	925	934	-13	4	403	372	-5	6	292	333	11	9	878	885
-13	2	355	348	-10	4	305	367	-4	6	623	647	12	9	880	903
-12	2	1051	1050	-9	4	957	930	-2	6	470	469	14	9	591	580
-11	2	951	966	-8	4	662	685	2	6	532	562	-7	10	241	195
-8	2	707	743	-7	4	883	860	4	6	281	203	-6	10	384	327
-6	2	835	838	-6	4	299	245	5	6	842	853	-5	10	457	429
-4	2	897	908	-5	4	631	649	6	6	766	725	-4	10	214	191
-3	2	1112	1161	-4	4	815	820	7	6	628	630	-2	10	312	278
-1	2	336	331	-2	4	1294	1363	9	6	313	239	5	10	552	546
0	2	415	471	-1	4	412	400	12	6	388	361	6	10	596	553
1	2	398	435	1	4	1624	1584	13	6	994	925	7	10	380	372
3	2	559	541	2	4	462	425	15	6	748	718	9	10	294	321
5	2	560	524	3	4	1408	1323	16	6	273	214	11	10	263	276
6	2	641	602	4	4	947	957	18	6	717	695	-3	11	615	620
7	2	989	1047	6	4	1190	1141	-13	7	205	206	-2	11	238	209
8	2	1272	1324	8	4	512	403	-11	7	349	379	-1	11	952	945
10	2	1231	1314	9	4	1053	1075	-8	7	354	301	0	11	683	721
11	2	878	898	11	4	710	736	-7	7	570	555	2	11	616	601
13	2	397	374	13	4	382	378	-5	7	467	463	3	11	463	480
14	2	1116	1157	14	4	933	935	-3	7	819	821	5	11	426	403
15	2	284	259	16	4	453	434	0	7	540	531	6	11	208	234
16	2	1683	1692	17	4	369	387	1	7	348	336	7	11	554	590
17	2	667	687	20	4	539	536	2	7	397	429				
18	2	1016	1046	-15	5	443	474	3	7	379	465	**L = -10****	0	819	835
19	2	393	347	-14	5	226	227	4	7	499	501	-12	0	1227	1256
20	2	351	350	-12	5	526	538	5	7	489	511	-10	0	1114	1041
-16	3	358	286	-10	5	411	468	6	7	519	444	-8	0	270	325
-15	3	827	837	-9	5	630	568	10	7	348	354	-6	0	661	634
-14	3	918	899	-8	5	258	197	11	7	784	777	-4	0	738	762
-13	3	509	516	-7	5	443	459	12	7	622	616	0	0	1477	1422
-12	3	264	117	-6	5	293	359	13	7	265	233	2	0	2417	2494
-11	3	291	316	-5	5	786	767	14	7	763	734	6	0	485	366
-10	3	881	863	-4	5	526	563	-11	8	372	374	8	0	1081	1119
-9	3	689	711	-3	5	1782	1809	-10	8	656	645	10	0	1530	1596
-7	3	813	801	-1	5	1437	1381	-5	8	267	146	12	0	889	916
-6	3	463	427	0	5	847	831	-4	8	448	450	16	0	1028	1114
-5	3	727	807	2	5	919	848	-3	8	274	302	18	0	441	494
-3	3	256	241	3	5	329	182	-2	8	746	646	20	0	268	280
				4	5	463	479	0	8	1041	1002	-17	1	269	268

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L = -10****			19	2	252	293	16	4	489	464	10	7	866	81
-16	1	324	278	21	2	239	166	18	4	428	507	-9	7	574	49
-14	1	430	392	-17	3	258	260	19	4	626	597	-8	7	399	39
-13	1	513	496	-15	3	231	272	-16	5	231	227	-6	7	954	90
-12	1	339	268	-14	3	260	279	-15	5	488	471	-5	7	333	33
-11	1	611	664	-13	3	527	527	-14	5	307	323	-3	7	330	35
-9	1	600	567	-12	3	1057	1085	-13	5	262	295	-1	7	623	61
-8	1	751	765	-11	3	780	790	-12	5	267	251	0	7	377	31
-7	1	876	935	-9	3	410	380	-10	5	668	669	2	7	421	42
-6	1	2162	2222	-8	3	774	762	-8	5	468	445	3	7	1046	95
-5	1	221	200	-4	3	771	776	-7	5	955	1020	4	7	762	71
-4	1	1070	1144	-3	3	702	698	-6	5	1084	1077	5	7	1399	137
-3	1	226	292	-1	3	379	349	-5	5	1303	1303	6	7	660	69
-2	1	830	802	0	3	1151	1193	-4	5	675	752	7	7	667	67
-1	1	664	689	1	3	423	437	-3	5	1682	1682	8	7	320	33
0	1	472	516	2	3	393	416	-1	5	456	373	9	7	307	26
1	1	1189	1206	3	3	601	503	2	5	1720	1705	11	7	713	71
2	1	373	422	5	3	767	733	3	5	1772	1725	12	7	1506	144
4	1	1393	1325	6	3	533	609	4	5	1228	1227	14	7	630	56
5	1	451	513	7	3	1030	1058	5	5	1048	1009	16	7	248	14
6	1	379	334	8	3	540	466	6	5	696	658	17	7	663	65
7	1	644	671	9	3	813	850	9	5	613	536	-9	8	806	76
8	1	282	195	10	3	465	498	10	5	633	614	-5	8	551	54
9	1	1647	1663	11	3	1361	1420	11	5	537	591	-3	8	353	33
10	1	454	447	12	3	861	907	14	5	890	845	-1	8	441	41
12	1	452	535	13	3	785	810	15	5	301	232	0	8	398	36
15	1	852	880	14	3	755	781	16	5	304	345	3	8	286	27
17	1	1080	1105	15	3	1166	1268	17	5	455	465	5	8	1352	137
18	1	502	497	16	3	590	583	18	5	546	512	7	8	760	80
21	1	244	270	17	3	385	430	-13	6	380	351	11	8	1703	167
-16	2	383	396	18	3	766	827	-12	6	431	435	13	8	1650	161
-15	2	666	669	19	3	874	895	-11	6	312	253	14	8	308	27
-14	2	309	298	-16	4	589	566	-10	6	713	765	15	8	280	27
-13	2	1216	1202	-15	4	496	491	-9	6	510	495	-10	9	534	56
-12	2	589	544	-14	4	525	471	-8	6	805	784	-9	9	418	44
-11	2	670	694	-11	4	958	989	-7	6	397	395	-8	9	718	74
-10	2	798	825	-10	4	440	465	-5	6	400	425	-6	9	580	56
-9	2	757	730	-8	4	581	619	-4	6	1757	1718	-5	9	355	42
-8	2	489	398	-6	4	421	347	-3	6	274	161	-3	9	464	51
-7	2	912	938	-5	4	299	232	-2	6	1942	1928	-2	9	346	29
-5	2	1363	1355	-4	4	524	520	0	6	856	811	-1	9	706	72
-3	2	572	565	-3	4	598	593	1	6	850	828	1	9	308	36
-2	2	871	840	-2	4	514	547	2	6	567	611	2	9	580	54
-1	2	992	965	-1	4	416	436	3	6	394	409	3	9	781	73
0	2	369	391	2	4	351	406	4	6	1234	1175	4	9	630	61
1	2	856	856	3	4	1350	1286	5	6	1030	996	5	9	899	88
3	2	1569	1388	4	4	1381	1365	6	6	876	875	-6	9	958	92
4	2	355	292	5	4	307	279	7	6	512	506	7	9	771	76
6	2	1237	1300	7	4	389	310	8	6	730	720	8	9	588	57
7	2	1352	1427	8	4	898	858	9	6	805	760	11	9	332	31
8	2	710	741	9	4	330	343	10	6	317	368	12	9	955	97
10	2	265	261	10	4	1518	1556	13	6	593	638	14	9	425	40
13	2	333	335	11	4	888	881	15	6	285	306	-8	10	301	29
14	2	795	874	12	4	474	522	16	6	304	240	-7	10	366	42
16	2	427	420	13	4	971	1041	19	6	468	468	-6	10	649	65
17	2	676	683	14	4	706	765	-12	7	556	530	-5	10	656	64
18	2	435	470	15	4	787	890	-11	7	750	759	-4	10	933	95

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
**L = -10****															
-2	10	996	1029	3	1	763	715	-3	3	1161	1196	-3	5	1626	1601
-1	10	279	263	4	1	802	770	1	3	785	775	-2	5	586	635
0	10	674	744	5	1	722	707	2	3	1498	1384	-1	5	1397	1379
1	10	692	752	6	1	1618	1679	3	3	532	499	0	5	1180	1173
2	10	328	270	7	1	674	696	5	3	1380	1296	1	5	615	598
3	10	222	299	8	1	1123	1140	6	3	740	715	3	5	1183	1119
4	10	723	763	9	1	844	793	7	3	1111	1128	4	5	2373	2380
6	10	607	571	10	1	417	469	9	3	1774	1843	5	5	491	473
8	10	367	367	11	1	1273	1282	10	3	485	534	6	5	359	378
9	10	540	570	12	1	471	418	12	3	627	601	7	5	625	656
10	10	458	425	14	1	416	385	13	3	400	424	9	5	488	502
-5	11	504	514	15	1	759	842	14	3	1282	1311	11	5	858	855
-4	11	260	201	16	1	787	804	15	3	998	1023	12	5	1106	1168
-3	11	555	543	17	1	683	722	16	3	770	783	14	5	347	407
-2	11	258	245	18	1	965	968	17	3	582	515	15	5	301	391
-1	11	320	304	19	1	333	301	19	3	486	436	19	5	527	545
0	11	316	330	20	1	294	275	21	3	395	411	20	5	678	668
1	11	203	184	22	1	274	321	-16	4	466	459	-16	6	351	372
2	11	839	841	-17	2	396	371	-15	4	573	567	-15	6	224	219
3	11	703	672	-15	2	244	249	-13	4	522	513	-12	6	465	430
4	11	348	366	-14	2	460	436	-12	4	456	475	-11	6	308	299
5	11	429	436	-12	2	481	439	-11	4	318	284	-8	6	379	375
6	11	504	546	-11	2	616	618	-10	4	650	677	-5	6	767	778
**L = -9****				-10	2	413	411	-9	4	916	965	-4	6	848	861
-15	0	797	784	-9	2	558	586	-8	4	903	896	-3	6	1610	1541
-13	0	830	806	-8	2	285	229	-7	4	1639	1699	-2	6	487	460
-9	0	777	789	-7	2	537	532	-6	4	386	413	-1	6	1438	1410
-7	0	1888	1910	-6	2	506	475	-5	4	470	429	0	6	288	297
-5	0	2505	2495	-5	2	689	717	-4	4	1085	1093	2	6	529	453
-3	0	796	738	-4	2	326	307	-3	4	312	276	3	6	1589	1554
-1	0	3000	3030	-3	2	994	1013	-2	4	1297	1336	5	6	1924	1861
1	0	1458	1424	-2	2	660	633	0	4	498	518	6	6	972	878
3	0	1155	1123	-1	2	938	929	1	4	1942	1884	7	6	945	887
5	0	809	834	0	2	736	755	2	4	526	399	9	6	361	364
7	0	1493	1583	2	2	895	929	3	4	531	525	11	6	574	541
9	0	737	756	2	2	933	904	4	4	663	645	13	6	1315	1256
11	0	364	303	2	2	1167	1138	4	4	1238	1166	15	6	517	456
15	0	627	680	6	2	1678	1736	6	4	295	259	18	6	655	638
17	0	1328	1279	7	2	1942	2067	7	4	853	908	19	6	407	409
19	0	808	773	8	2	274	258	8	4	611	545	19	6	613	586
21	0	498	505	9	2	1135	1223	9	4	771	756	-13	7	261	271
-16	1	421	414	10	2	618	595	10	4	359	410	-12	7	1079	1053
-14	1	267	254	11	2	758	740	11	4	348	412	-11	7	303	341
-13	1	953	975	13	2	1292	1287	12	4	1144	1097	-10	7	905	891
-12	1	468	431	14	2	473	470	15	4	555	563	-9	7	725	682
-11	1	541	519	15	2	1386	1440	16	4	586	553	-7	7	904	915
-9	1	571	579	16	2	526	545	18	4	586	553	-5	7	476	496
-8	1	529	523	17	2	458	443	20	4	1020	1014	-4	7	769	771
-7	1	398	349	18	2	262	333	-15	5	414	420	-3	7	542	520
-6	1	227	283	21	2	836	830	-14	5	335	302	-2	7	350	304
-4	1	740	798	-17	3	379	342	-13	5	289	214	-1	7	271	248
-2	1	1325	1321	-16	3	570	605	-12	5	303	258	1	7	671	735
-1	1	648	667	-15	3	1358	1355	-11	5	784	768	3	7	483	518
0	1	1349	1312	-14	3	566	590	-10	5	408	384	4	7	418	391
1	1	2196	2143	-11	3	439	460	-9	5	970	1003	5	7	1221	1170
2	1	349	322	-10	3	446	409	-8	5	541	543	6	7	391	348
				-9	3	1144	1129	-6	5	813	815	8	7	938	860
				-6	3			-4	5			10	7		

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-9****		13	10	543	578	8	1	1294	1281	-1	3	353	364
12	7	1165	1159	-6	11	524	507	9	1	1394	1418	0	3	968	946
13	7	579	539	-3	11	605	584	10	1	661	757	2	3	472	188
14	7	592	616	-2	11	589	623	12	1	324	319	3	3	1634	1630
16	7	358	386	-1	11	1036	1024	15	1	968	976	4	3	874	882
-13	8	229	121	0	11	766	819	16	1	411	381	5	3	326	341
-12	8	951	975	1	11	371	363	18	1	1106	1060	6	3	907	905
-11	8	244	182	4	11	722	729	21	1	619	642	7	3	340	358
-10	8	1281	1224	6	11	440	416	22	1	834	818	8	3	902	899
-8	8	795	840	7	11	379	410	-19	2	426	433	9	3	1280	1329
-6	8	377	263	9	11	235	248	-18	2	415	424	10	3	1006	1081
-4	8	607	549	10	11	232	172	-17	2	311	275	11	3	1454	1598
-2	8	527	516	1	12	803	835	-16	2	372	354	12	3	648	673
0	8	854	837	4	12	296	274	-15	2	1135	1121	13	3	476	442
2	8	808	843					-13	2	1579	1598	16	3	1356	1408
4	8	329	363	-18	0	337	297	-12	2	853	896	17	3	328	317
5	8	268	192	-14	0	359	371	-11	2	652	729	18	3	531	498
8	8	625	662	-12	0	748	775	-10	2	596	609	19	3	905	940
12	8	593	529	-10	0	359	319	-9	2	819	836	20	3	466	434
14	8	1130	1109	-8	0	1763	1794	-7	2	939	941	21	3	334	311
16	8	589	543	-6	0	1804	1852	-6	2	380	378	-16	4	474	440
-11	9	585	598	-4	0	1027	1005	-5	2	1336	1348	-15	4	247	198
-9	9	881	845	-2	0	969	914	-4	2	930	942	-12	4	329	314
-8	9	410	390	0	0	4496	4672	-2	2	256	271	-11	4	578	558
-6	9	295	278	2	0	3699	3741	0	2	884	905	-10	4	994	988
-5	9	746	742	4	0	967	978	1	2	643	537	-9	4	1187	1230
-4	9	512	496	6	0	1718	1663	2	2	1199	1163	-8	4	357	401
-3	9	468	458	8	0	1396	1491	3	2	541	543	-6	4	531	586
-2	9	336	377	10	0	845	792	4	2	581	546	-5	4	456	457
-1	9	826	789	12	0	1058	1124	8	2	1590	1636	-4	4	438	437
3	9	926	951	14	0	441	453	9	2	1421	1493	-3	4	418	393
4	9	1043	1010	16	0	1118	1123	10	2	994	1064	-2	4	1054	1040
5	9	961	916	18	0	567	561	11	2	557	513	-1	4	1231	1251
6	9	1059	987	20	0	343	350	12	2	648	662	0	4	758	752
8	9	405	378	-17	1	252	182	13	2	698	719	1	4	418	400
9	9	371	326	-16	1	480	543	15	2	1398	1419	2	4	1913	1826
10	9	633	597	-14	1	1139	1171	16	2	441	421	3	4	1611	1568
12	9	1014	1013	-12	1	732	754	17	2	1599	1614	4	4	1532	1514
13	9	801	783	-11	1	939	951	18	2	1057	1007	5	4	1490	1406
14	9	594	576	-10	1	290	274	19	2	289	393	6	4	510	516
15	9	483	419	-9	1	311	291	21	2	434	484	7	4	271	317
-9	10	347	296	-8	1	1086	1111	22	2	265	250	8	4	1456	1446
-8	10	385	379	-7	1	1379	1436	-17	3	785	758	9	4	764	779
-7	10	206	172	-6	1	2201	2200	-16	3	846	825	10	4	1624	1693
-6	10	342	362	-5	1	795	795	-15	3	447	448	11	4	775	756
-4	10	423	420	-4	1	1473	1474	-14	3	633	647	13	4	1079	1116
-3	10	755	744	-3	1	997	955	-12	3	722	717	14	4	396	334
-2	10	517	465	-2	1	440	480	-11	3	820	858	15	4	352	363
-1	10	614	623	-1	1	1621	1595	-10	3	730	747	17	4	595	605
1	10	279	252	0	1	301	373	-9	3	561	611	18	4	640	563
2	10	408	374	1	1	1443	1497	-8	3	1636	1614	19	4	444	380
3	10	675	691	2	1	566	530	-7	3	798	789	20	4	246	235
5	10	1141	1144	3	1	1101	1051	-6	3	484	438	21	4	313	240
6	10	797	814	4	1	1106	1193	-5	3	742	710	-17	5	240	194
7	10	1071	1072	5	1	474	407	-4	3	353	414	-16	5	480	470
11	10	576	607	6	1	306	258	-3	3	1383	1382	-15	5	444	484
12	10	236	179	7	1	1879	1960	-2	3	539	567	-14	5	532	542

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-8****													
-13	5	642	668	12	7	1490	1416	1	11	599	584	6	1	554	599
-11	5	302	302	13	7	1098	1000	2	14	696	690	7	1	431	469
-6	5	1009	1069	17	7	599	583	3	11	567	565	8	1	903	912
-5	5	1235	1316	18	7	534	489	4	11	351	340	9	1	309	254
-4	5	715	727	-14	8	216	160	5	11	225	164	10	1	1400	1384
-3	5	759	829	-12	8	390	412	6	11	825	871	11	1	856	898
-2	5	1737	1745	-11	8	818	767	7	11	281	310	12	1	332	332
1	5	694	678	-7	8	271	297	9	11	253	228	13	1	519	495
2	5	674	684	-4	8	362	377	10	11	400	428	15	1	670	711
3	5	369	416	-3	8	1025	1053	11	11	214	236	16	1	1507	1465
4	5	709	631	0	8	581	586	-3	12	478	456	18	1	711	733
6	5	1511	1537	3	8	411	403	-2	12	534	565	22	1	251	182
7	5	294	344	4	8	369	359	-1	12	677	688	-19	2	255	223
9	5	632	667	5	8	1349	1299	0	12	781	783	-17	2	757	753
10	5	340	293	7	8	796	767	1	12	515	528	-16	2	497	522
12	5	483	540	11	8	1672	1616	2	12	880	910	-15	2	520	492
13	5	750	746	13	8	809	770	3	12	448	490	-14	2	778	774
14	5	958	966	-12	9	231	205	4	12	321	308	-13	2	319	323
17	5	506	437	-11	9	491	511	5	12	366	363	-12	2	722	740
19	5	507	464	-9	9	496	502					-10	2	568	575
-16	6	350	361	-8	9	253	297	-17	0	583	557	-9	2	959	991
-15	6	405	395	-6	9	362	374	-15	0	787	734	-8	2	1064	1113
-12	6	996	961	-5	9	374	311	-13	0	1190	1123	-7	2	850	882
-11	6	666	686	-4	9	705	697	-11	0	367	341	-6	2	1293	1351
-10	6	1242	1276	-2	9	715	725	-9	0	1048	1021	-5	2	1393	1383
-9	6	349	268	-1	9	735	727	-5	0	1558	1584	-4	2	905	885
-8	6	517	487	1	9	253	181	-3	0	307	274	-3	2	365	300
-7	6	712	706	3	9	322	319	-1	0	1729	1664	-1	2	284	277
-6	6	534	524	4	9	666	660	1	0	2298	2403	0	2	1388	1392
-4	6	1206	1218	6	9	534	590	3	0	372	329	1	2	708	688
-3	6	341	394	8	9	455	412	5	0	591	604	2	2	1658	1492
-2	6	706	680	10	9	335	353	7	0	353	285	5	2	1387	1503
-1	6	572	663	11	9	440	355	9	0	1956	2022	6	2	632	741
0	6	378	373	12	9	819	796	11	0	363	319	7	2	1336	1329
1	6	1083	1058	13	9	984	927	17	0	1403	1457	8	2	1535	1570
3	6	538	581	14	9	335	323	19	0	412	410	9	2	290	329
6	6	565	574	-10	10	806	831	21	0	264	350	10	2	347	344
7	6	784	760	-8	10	479	497	-16	1	421	413	11	2	340	315
8	6	355	343	-7	10	461	479	-15	1	605	566	12	2	661	706
9	6	663	628	-6	10	616	595	-13	1	542	558	13	2	674	684
11	6	345	325	-5	10	278	219	-12	1	626	598	14	2	482	467
12	6	602	582	-4	10	620	648	-10	1	671	737	18	2	500	546
14	6	770	767	-2	10	259	280	-9	1	218	208	19	2	685	686
15	6	713	660	0	10	564	573	-8	1	246	261	20	2	304	306
19	6	561	522	1	10	678	630	-7	1	1704	1690	21	2	538	519
-11	7	456	501	2	10	409	442	-6	1	693	681	22	2	311	302
-9	7	568	546	6	10	548	551	-5	1	889	944	-19	3	627	624
-6	7	304	285	7	10	485	462	-4	1	244	264	-18	3	431	438
-4	7	1053	1067	8	10	225	109	-3	1	777	763	-17	3	427	398
-1	7	829	845	9	10	546	541	-2	1	1367	1386	-14	3	1400	1426
0	7	475	448	10	10	268	297	-1	1	1148	1111	-13	3	854	842
2	7	260	159	12	10	414	439	0	1	341	386	-12	3	561	552
3	7	872	835	-6	11	466	512	1	1	2702	2659	-11	3	752	726
4	7	1627	1581	-5	11	833	855	2	1	915	917	-10	3	467	471
6	7	323	323	-4	11	503	491	3	1	1563	1547	-9	3	869	872
8	7	439	442	-2	11	1082	1059	4	1	728	751	-7	3	500	448
				-1	11	410	429	5	1	787	763	-6	3	716	770

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-7****		-10	5	335	412	-12	7	887	881	6	9	1021	1035
-4	3	491	463	-9	5	854	848	-11	7	787	779	8	9	536	556
-3	3	731	763	-8	5	1251	1278	-10	7	976	956	10	9	687	635
-1	3	1161	1167	-7	5	478	414	-9	7	1119	1163	11	9	698	676
1	3	1524	1460	-5	5	679	703	-7	7	303	286	12	9	413	433
2	3	397	381	-4	5	1848	1916	-5	7	1116	1130	13	9	1152	1121
3	3	435	363	-3	5	572	564	-4	7	714	667	16	9	589	554
4	3	413	254	-2	5	615	573	-3	7	316	267	-11	10	830	798
6	3	922	946	-1	5	303	321	-2	7	1385	1346	-8	10	222	225
7	3	1308	1338	0	5	944	892	0	7	333	311	-7	10	278	226
8	3	655	652	1	5	1165	1074	2	7	946	976	-6	10	842	832
9	3	844	859	2	5	999	902	3	7	354	290	-5	10	686	683
10	3	1010	1049	3	5	1652	1621	4	7	1123	1102	-4	10	520	509
11	3	1244	1310	4	5	2718	2677	5	7	1398	1355	-3	10	1414	1471
12	3	326	335	5	5	485	505	6	7	1488	1442	-2	10	588	620
13	3	626	655	7	5	321	274	8	7	370	313	-1	10	1139	1126
14	3	1724	1784	8	5	471	459	10	7	936	898	0	10	811	822
15	3	632	586	9	5	878	850	11	7	1004	963	2	10	747	780
16	3	640	593	10	5	640	576	12	7	408	321	3	10	904	930
17	3	528	449	11	5	852	844	13	7	1501	1480	5	10	1106	1071
18	3	793	804	12	5	945	933	16	7	353	364	6	10	378	382
19	3	711	696	13	5	342	263	18	7	360	288	7	10	751	779
22	3	692	716	15	5	1041	1077	19	7	888	834	9	10	274	167
-18	4	620	660	16	5	320	336	-15	8	276	270	10	10	546	543
-17	4	311	323	19	5	498	488	-13	8	264	258	11	10	617	612
-16	4	605	646	-17	6	227	258	-12	8	781	752	-9	11	538	491
-15	4	727	732	-16	6	478	460	-10	8	887	886	-8	11	582	595
-13	4	321	302	-14	6	287	290	-8	8	805	774	-5	11	560	553
-12	4	1094	1084	-13	6	405	371	-6	8	794	830	-4	11	786	774
-10	4	657	674	-12	6	416	456	-5	8	432	423	-2	11	579	548
-7	4	1226	1235	-11	6	848	860	-3	8	301	274	-1	11	491	476
-6	4	699	785	-10	6	398	374	-2	8	355	413	1	11	573	613
-4	4	1078	1073	-9	6	534	552	-1	8	356	341	2	11	633	646
-2	4	914	842	-8	6	326	339	0	8	390	410	3	11	847	850
-1	4	490	468	-7	6	333	271	2	8	758	775	4	11	913	931
0	4	584	620	-6	6	791	787	4	8	812	822	5	11	421	395
1	4	474	435	-5	6	1390	1358	6	8	1076	1045	9	11	493	480
2	4	1395	1368	-4	6	911	873	8	8	551	552	10	11	390	408
3	4	1338	1313	-3	6	2689	2636	10	8	678	626	11	11	221	204
4	4	302	290	-2	6	623	642	12	8	2124	2070	-5	12	210	206
5	4	273	331	-1	6	1465	1427	13	8	324	261	-3	12	234	216
7	4	1473	1485	0	6	674	675	14	8	1246	1201	-1	12	340	328
8	4	308	384	2	6	673	698	16	8	435	384	2	12	376	396
9	4	766	806	3	6	1803	1804	-13	9	638	588	3	12	626	671
10	4	1745	1737	5	6	1727	1695	-12	9	809	832	7	12	627	658
11	4	1421	1458	6	6	576	585	-11	9	663	617				
12	4	1219	1262	7	6	509	493	-10	9	580	581	**L =	-6****	259	219
13	4	327	281	8	6	477	454	-9	9	944	928	-18	0	368	335
14	4	449	438	10	6	516	456	-5	9	696	737	-16	0	1004	1054
15	4	1099	1090	11	6	301	321	-4	9	741	775	-12	0	230	188
16	4	484	468	12	6	861	824	-2	9	763	724	-8	0	2131	2223
17	4	585	538	13	6	573	544	-1	9	650	632	-6	0	2838	2837
18	4	754	723	14	6	440	364	0	9	515	519	-4	0	823	853
20	4	1033	1022	16	6	302	291	1	9	341	369	-2	0	1278	1250
21	4	523	510	20	6	788	709	2	9	328	346	0	0	3427	3542
-16	5	398	372	-15	7	481	464	4	9	919	936	2	0	1566	1590
-11	5	1106	1100	-13	7	833	768	5	9	1425	1435	4	0	999	1021



H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-6****													
6	0	1860	1851	1	2	2242	2186	-11	4	656	604	19	5	628	609
8	0	1382	1251	2	2	1528	1476	-10	4	1151	1114	20	5	351	358
12	0	732	781	3	2	626	596	-9	4	1628	1605	21	5	468	490
14	0	571	586	4	2	260	145	-8	4	1048	1062	-16	6	438	434
16	0	513	504	5	2	991	965	-7	4	327	328	-15	6	506	532
18	0	895	913	6	2	1288	1336	-6	4	1824	1805	-12	6	522	533
20	0	523	552	7	2	1362	1406	-5	4	1119	1197	-11	6	567	581
22	0	372	368	8	2	1866	1880	-4	4	248	235	-10	6	436	457
-19	1	302	275	9	2	2349	2418	-3	4	1256	1321	-7	6	706	712
-17	1	259	212	10	2	1496	1481	-2	4	841	778	-5	6	1006	1002
-16	1	342	264	11	2	579	616	-1	4	1216	1184	-4	6	727	539
-15	1	616	601	12	2	829	859	0	4	672	687	-3	6	606	542
-14	1	1441	1409	13	2	792	838	2	4	1523	1532	-2	6	1437	1453
-12	1	901	923	14	2	866	846	3	4	962	915	-1	6	1010	970
-11	1	838	842	15	2	2000	2025	4	4	444	377	0	6	297	311
-10	1	552	539	17	2	1298	1297	5	4	1625	1636	-1	6	629	606
-9	1	883	881	18	2	568	597	6	4	430	441	2	6	943	947
-8	1	336	318	21	2	601	520	7	4	672	701	3	6	1149	1086
-7	1	1666	1599	-19	3	310	261	8	4	318	374	4	6	1947	1892
-6	1	798	820	-18	3	592	541	9	4	528	483	5	6	688	680
-5	1	1034	1034	-17	3	603	620	10	4	506	533	6	6	1195	1178
-4	1	878	886	-16	3	1099	1097	11	4	445	494	7	6	1152	1067
-3	1	657	670	-15	3	1303	1309	12	4	559	515	9	6	427	383
-1	1	2206	2229	-14	3	251	257	13	4	667	682	12	6	1105	1108
0	1	2301	2299	-13	3	723	742	14	4	359	380	14	6	1065	1012
1	1	1845	1786	-11	3	829	842	15	4	728	725	15	6	456	467
2	1	1392	1320	-10	3	802	805	16	4	539	522	17	6	293	291
3	1	720	713	-8	3	1061	1061	19	4	1198	1174	19	6	340	306
4	1	485	549	-7	3	1384	1407	21	4	446	441	20	6	830	791
6	1	414	448	-5	3	1236	1218	-17	5	347	348	-17	7	617	613
7	1	2501	2552	-3	3	1161	1191	-16	5	287	341	-16	7	393	375
8	1	1449	1473	-2	3	712	713	-14	5	449	491	-12	7	852	871
10	1	1905	1940	-1	3	503	521	-13	5	972	963	-11	7	275	245
12	1	325	331	1	3	901	903	-10	5	918	935	-10	7	518	496
14	1	473	465	2	3	555	532	-9	5	701	680	-9	7	556	579
16	1	270	287	3	3	1280	1283	-8	5	440	400	-8	7	1175	1173
17	1	1334	1313	4	3	828	783	-7	5	678	698	-7	7	452	468
18	1	1032	980	5	3	1329	1319	-5	5	280	302	-6	7	708	766
21	1	628	606	6	3	698	606	-4	5	1129	1168	-4	7	1973	1916
22	1	796	801	7	3	256	234	-3	5	453	466	-3	7	1078	1086
-19	2	251	234	8	3	1646	1691	-2	5	2759	2778	-2	7	494	460
-18	2	366	358	9	3	770	814	-1	5	1700	1667	-1	7	259	218
-17	2	353	370	10	3	629	607	0	5	555	565	0	7	724	705
-16	2	357	376	11	3	1776	1800	1	5	512	507	2	7	283	299
-15	2	1089	1108	12	3	243	161	2	5	270	318	4	7	940	931
-13	2	1014	1027	13	3	434	415	3	5	1061	1098	5	7	1246	1186
-12	2	900	946	14	3	916	918	4	5	774	756	6	7	393	446
-11	2	291	228	15	3	684	704	5	5	1192	1153	7	7	498	495
-9	2	279	211	16	3	1318	1380	6	5	1335	1302	8	7	498	455
-8	2	347	367	18	3	595	567	9	5	531	603	9	7	684	630
-6	2	1719	1753	19	3	557	560	10	5	568	625	11	7	656	585
5	2	473	495	20	3	719	712	11	5	848	820	13	7	1424	1334
-4	2	1171	1142	21	3	595	629	12	5	317	262	14	7	614	615
-3	2	547	549	22	3	273	253	13	5	903	915	15	7	528	557
-1	2	932	909	-17	4	875	876	14	5	307	228	17	7	513	434
0	2	1752	1766	-14	4	918	889	17	5	288	185	19	7	265	219
				-13	4	387	388	18	5	378	409	-15	8	771	734



H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
		**L = -6****		7	10	728	734	-6	1	583	598	16	2	1315	1357
-14	8	293	322	9	10	248	262	-5	1	1852	1831	18	2	1023	1041
-13	8	571	591	10	10	388	333	-4	1	203	128	19	2	1179	1140
-12	8	368	349	11	10	321	305	-3	1	270	279	20	2	524	541
-11	8	1518	1489	12	10	714	741	-2	1	772	804	21	2	478	435
-9	8	845	826	13	10	228	270	-1	1	463	440	22	2	958	914
-7	8	472	469	14	10	711	693	0	1	3106	3088	-20	3	224	235
-6	8	306	255	-7	11	733	776	1	1	674	707	-19	3	663	679
-5	8	1101	1142	-5	11	477	462	2	1	1681	1606	-18	3	934	953
-3	8	803	786	-4	11	378	405	3	1	1588	1605	-17	3	442	400
-1	8	372	350	-3	11	690	668	4	1	239	285	-16	3	351	353
2	8	269	280	-2	11	1381	1377	5	1	797	805	-15	3	780	766
3	8	864	825	-1	11	901	907	6	1	653	641	-14	3	411	399
5	8	481	477	0	11	393	402	7	1	938	922	-13	3	1230	1277
6	8	268	220	1	11	464	458	8	1	3240	3339	-12	3	274	237
7	8	590	540	5	11	734	730	9	1	1628	1692	-11	3	345	310
11	8	492	474	6	11	960	912	10	1	205	244	-10	3	999	1027
13	8	785	830	7	11	385	385	11	1	728	747	-9	3	1975	2066
17	8	759	715	8	11	477	475	12	1	263	213	-8	3	836	818
-14	9	304	250	11	11	363	343	13	1	470	474	-7	3	376	405
-13	9	215	147	12	11	458	412	14	1	254	112	-6	3	1032	953
-12	9	1063	1090	-6	12	577	613	16	1	1183	1171	-5	3	501	458
-10	9	594	600	-3	12	813	800	17	1	783	846	-4	3	478	410
-9	9	352	368	-2	12	277	288	20	1	332	279	-3	3	880	857
-8	9	246	233	-1	12	491	494	21	1	686	689	-2	3	531	526
-6	9	528	517	0	12	801	775	22	1	307	334	-1	3	1678	1684
-5	9	388	402	1	12	493	512	-20	2	554	566	1	3	269	269
-4	9	949	922	2	12	496	498	-17	2	1047	1057	2	3	1031	999
-3	9	483	520	3	12	291	334	-16	2	1458	1464	3	3	595	547
-2	9	570	605	5	12	317	312	-15	2	476	453	4	3	1135	1108
0	9	511	510	6	12	205	188	-14	2	1618	1636	5	3	293	280
2	9	333	339	8	12	362	401	-13	2	612	584	6	3	1742	1765
4	9	286	338			**L = -5****		-12	2	1020	1006	7	3	1139	1131
5	9	943	909	-13	0	913	895	-11	2	807	809	8	3	917	901
6	9	487	496	-11	0	1323	1312	-9	2	804	785	9	3	1065	1080
7	9	341	259	-9	0	192	173	-8	2	1752	1734	10	3	1992	2079
8	9	469	491	-7	0	1743	1780	-7	2	1092	1057	11	3	1649	1692
9	9	366	379	-5	0	596	617	-6	2	1667	1638	12	3	400	372
10	9	320	296	-3	0	1151	1147	-5	2	1137	1099	14	3	1338	1335
11	9	1258	1225	-1	0	2298	2237	-4	2	934	939	15	3	660	611
12	9	265	295	1	0	4940	5252	-3	2	1156	1155	16	3	274	267
13	9	1089	1053	7	0	2728	2656	-2	2	742	715	17	3	809	763
14	9	923	892	9	0	2916	2941	0	2	266	339	18	3	1035	1021
-11	10	244	205	15	0	645	610	2	2	256	174	19	3	347	332
-10	10	537	537	17	0	1235	1126	3	2	768	761	20	3	559	531
-9	10	318	323	21	0	358	326	4	2	331	316	-19	4	333	360
-8	10	346	356	-20	1	711	704	5	2	1611	1656	-17	4	304	277
-7	10	364	364	-19	1	446	411	6	2	512	511	-16	4	260	270
-6	10	274	211	-18	1	462	491	7	2	1443	1414	-15	4	470	517
-5	10	574	582	-17	1	453	400	8	2	913	939	-14	4	489	529
-4	10	728	734	-15	1	1203	1241	9	2	208	111	-13	4	433	462
-2	10	514	541	-14	1	335	286	10	2	588	611	-12	4	930	946
-1	10	566	586	-13	1	561	530	11	2	1691	1750	-11	4	297	286
2	10	349	359	-10	1	1432	1385	12	2	528	544	-10	4	484	492
4	10	1134	1202	-9	1	701	676	13	2	373	326	-8	4	794	834
5	10	681	727	-8	1	1866	1836	14	2	686	672	-6	4	715	698
6	10	1596	1544	-7	1	2637	2680	15	2	454	414	-5	4	996	1029

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-5****													
-3	4	932	994	-16	6	315	329	-8	8	273	247	13	10	843	822
-2	4	1206	1183	-14	6	646	649	-7	8	444	378	14	10	366	326
-1	4	1074	1098	-13	6	1043	1088	-6	8	450	427	-10	11	214	239
0	4	633	657	-12	6	336	348	-5	8	533	534	-7	11	350	370
1	4	729	692	-11	6	989	1047	-4	8	805	773	-6	11	429	411
2	4	2021	1996	-9	6	640	673	-2	8	303	363	-5	11	888	918
3	4	2737	2778	-6	6	797	820	1	8	327	357	-4	11	781	804
4	4	1018	988	-5	6	1524	1546	2	8	539	515	-3	11	646	705
5	4	481	395	-4	6	599	603	4	8	1778	1787	0	11	588	627
6	4	623	591	-3	6	2293	2267	6	8	1099	1081	1	11	642	629
7	4	1871	1919	-1	6	888	884	8	8	621	583	2	11	1140	1166
9	4	1986	1966	0	6	746	697	9	8	532	515	3	11	643	615
10	4	1538	1563	1	6	343	64	10	8	934	905	4	11	454	392
11	4	1673	1742	2	6	603	583	12	8	1925	1889	5	11	875	963
12	4	141	1102	3	6	1290	1281	13	8	414	393	6	11	518	485
13	4	319	314	4	6	931	946	14	8	765	761	7	11	699	703
15	4	479	474	5	6	462	425	16	8	409	369	9	11	458	446
17	4	341	301	6	6	1387	1372	18	8	752	758	10	11	319	360
18	4	393	450	8	6	540	450	-18	9	383	404	-6	12	261	266
20	4	363	373	9	6	581	600	-12	9	894	895	-5	12	473	477
-19	5	585	617	10	6	288	257	-11	9	219	194	-3	12	366	329
-16	5	620	625	12	6	1031	1025	-10	9	641	609	-2	12	698	735
-15	5	273	323	13	6	541	563	-9	9	544	557	-1	12	834	866
-14	5	443	482	14	6	923	897	-4	9	311	259	1	12	548	588
-13	5	391	413	15	6	416	349	-3	9	813	828	2	12	743	758
-12	5	386	420	16	6	432	396	-2	9	865	937	3	12	950	993
-11	5	773	790	19	6	565	571	-1	9	293	272	4	12	373	345
-8	5	1182	1232	20	6	716	675	1	9	555	565	6	12	362	336
-6	5	688	694	-17	7	400	446	2	9	511	506	7	12	555	573
-5	5	949	970	-13	7	410	433	3	9	323	200	8	12	528	521
-4	5	823	910	-12	7	736	737	5	9	1298	1319	9	12	621	628
-3	5	1817	1851	-10	7	958	917	6	9	508	492				
-2	5	1359	1319	-9	7	485	478	7	9	309	226	**L =	-4****		
-1	5	960	946	-4	7	346	310	11	9	605	583	-20	0	247	303
0	5	755	719	-3	7	958	926	12	9	637	541	-16	0	1269	1290
1	5	248	136	-2	7	1220	1263	13	9	686	651	-14	0	565	580
2	5	1521	1508	-1	7	315	256	15	9	350	314	-10	0	683	679
3	5	722	741	1	7	595	588	16	9	619	545	-8	0	1906	1860
4	5	1558	1576	2	7	866	832	-13	10	513	516	-6	0	1781	1820
5	5	806	846	3	7	1611	1575	-12	10	277	213	-4	0	939	919
6	5	1589	1506	4	7	603	519	-11	10	1264	1322	-2	0	1762	1717
7	5	991	946	5	7	1669	1648	-9	10	489	467	0	0	2306	2162
8	5	1070	1054	6	7	944	966	-8	10	230	193	4	0	1770	1730
9	5	643	673	8	7	491	447	-7	10	471	530	6	0	338	284
10	5	1038	989	9	7	454	458	-6	10	795	798	8	0	1321	1322
11	5	584	553	10	7	346	332	-5	10	546	462	10	0	1927	1918
14	5	324	301	11	7	1325	1250	-4	10	413	322	12	0	327	323
15	5	796	766	12	7	735	731	-3	10	1253	1251	14	0	1101	1057
16	5	978	945	13	7	1133	1090	-1	10	1018	1084	16	0	1207	1173
17	5	459	451	14	7	639	626	0	10	520	506	18	0	1401	1393
18	5	411	413	16	7	783	710	1	10	311	266	20	0	937	889
20	5	306	243	18	7	625	641	2	10	491	527	-21	1	442	425
21	5	866	832	19	7	846	756	3	10	643	641	-19	1	260	247
-18	6	508	506	-16	8	308	288	6	10	264	259	-17	1	943	926
-17	6	264	301	-14	8	527	538	9	10	259	300	-16	1	550	516
				-13	8	408	349	10	10	341	296	-15	1	550	570
				-12	8	553	547	12	10	432	441	-14	1	685	676
												-13	1	323	296

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCA
	**L =	-4****		-16	3	332	301	1	4	517	572	-3	6	687	67
-9	1	881	925	-15	3	1667	1692	2	4	578	592	-2	6	1683	167
-8	1	1763	1780	-14	3	747	759	3	4	732	719	-1	6	758	80
-6	1	1412	1369	-13	3	744	743	4	4	1057	976	0	6	917	88
-5	1	1097	1094	-12	3	775	780	5	4	718	662	1	6	435	43
-3	1	414	388	-11	3	247	203	6	4	920	899	2	6	1679	166
-1	1	1795	1773	-10	3	223	135	7	4	543	576	3	6	842	89
0	1	3340	3345	-9	3	397	437	8	4	929	841	4	6	2979	298
1	1	1774	1714	-8	3	712	727	9	4	846	870	5	6	1183	115
2	1	2662	2710	-7	3	1734	1748	10	4	1366	1355	6	6	1110	110
3	1	878	861	-6	3	1040	1045	11	4	1525	1535	7	6	891	88
4	1	1762	1742	-5	3	1046	1077	12	4	1135	1125	8	6	385	37
5	1	802	758	-4	3	1126	1126	14	4	1303	1342	10	6	379	37
6	1	727	675	-3	3	618	616	15	4	949	977	12	6	1091	103
8	1	690	702	-2	3	252	315	16	4	593	610	13	6	516	45
9	1	1981	1960	-1	3	1578	1665	17	4	462	457	17	6	301	34
10	1	1726	1731	0	3	1417	1351	19	4	1672	1681	-18	7	451	44
11	1	339	296	1	3	1764	1672	21	4	508	491	-17	7	346	27
14	1	429	424	2	3	664	548	18	5	510	533	-16	7	733	75
15	1	286	361	3	3	1184	1154	-16	5	296	283	-15	7	335	35
17	1	1972	1920	4	3	1387	1370	-13	5	571	583	-14	7	451	47
21	1	351	387	5	3	315	281	-12	5	602	622	-13	7	789	78
22	1	504	429	6	3	1225	1201	-10	5	1822	1838	-12	7	1254	124
-21	2	533	556	7	3	1325	1343	-9	5	1586	1588	-11	7	812	86
-20	2	593	590	8	3	1350	1403	-7	5	662	636	-10	7	873	89
-18	2	282	321	9	3	794	742	-6	5	629	679	-8	7	987	10
-15	2	281	253	10	3	448	504	-5	5	1505	1548	-7	7	494	48
-14	2	691	702	11	3	281	308	-3	5	1579	1565	-6	7	1173	114
-12	2	652	670	12	3	645	610	-2	5	1491	1512	-5	7	1075	108
-11	2	508	572	13	3	1385	1418	-1	5	1482	1467	-4	7	1748	178
-10	2	1336	1273	14	3	1252	1233	1	5	395	367	-3	7	1702	17
-9	2	563	574	15	3	1329	1283	2	5	1153	1108	-2	7	269	3
-8	2	197	116	16	3	816	835	3	5	2519	2575	-1	7	353	3
7	2	1861	1892	17	3	380	331	4	5	899	856	0	7	475	4
6	2	2494	2524	18	3	1455	1376	5	5	447	443	1	7	240	2
-5	2	1226	1154	19	3	481	444	6	5	500	448	3	7	890	9
-4	2	303	271	20	3	400	480	7	5	309	231	4	7	268	2
-2	2	1048	1039	21	3	580	559	10	5	1136	1138	5	7	2240	22
0	2	1356	1346	22	3	260	211	11	5	1483	1478	6	7	1256	12
1	2	1353	1302	-20	4	383	363	12	5	436	433	7	7	633	6
2	2	1194	1152	-19	4	762	773	15	5	561	599	8	7	400	4
4	2	704	702	-17	4	1025	1029	16	5	329	280	9	7	744	6
5	2	754	737	-16	4	669	667	18	5	836	799	10	7	814	7
6	2	1712	1717	-14	4	1073	1119	20	5	559	538	11	7	843	8
7	2	1313	1338	-13	4	440	447	21	5	263	173	12	7	1389	13
8	2	760	768	-11	4	994	977	-18	6	250	262	13	7	607	6
9	2	1647	1692	-10	4	835	866	-17	6	285	234	14	7	635	6
11	2	264	254	-9	4	1351	1352	-16	6	282	221	15	7	513	4
12	2	691	687	-8	4	1722	1726	-15	6	296	310	16	7	311	3
13	2	738	796	-7	4	993	996	-13	6	559	591	18	7	349	3
14	2	1000	984	-6	4	990	991	-12	6	294	223	19	7	345	3
15	2	789	799	-5	4	399	398	-11	6	686	625	-16	8	273	2
16	2	411	401	-4	4	772	762	-10	6	397	338	-15	8	544	5
18	2	323	339	-3	4	1018	1036	-9	6	323	388	-14	8	388	4
19	2	311	368	-2	4	547	554	-6	6	720	706	-13	8	916	9
22	2	315	306	-1	4	605	596	-5	6	2310	2418	-11	8	1297	12
-18	3	887	892	0	4	538	546	-4	6	2627	2684	-9	8	882	8

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-4****		12	10	423	395	-16	1	575	571	2	2	796	724
-6	8	263	194	13	10	219	142	-15	1	1401	1398	3	2	724	736
-5	8	898	890	14	10	216	187	-13	1	828	782	5	2	353	367
-2	8	305	354	-11	11	259	224	-12	1	445	444	6	2	418	376
-1	8	429	400	-10	11	845	888	-11	1	348	328	7	2	2630	2699
0	8	342	298	-9	11	200	220	-10	1	429	408	8	2	2940	2992
1	8	526	558	-7	11	646	672	-9	1	218	225	10	2	862	913
2	8	561	613	-6	11	409	406	-8	1	2146	2248	11	2	1643	1705
5	8	952	903	-3	11	1028	1068	-7	1	1417	1402	12	2	1642	1623
6	8	295	282	-2	11	1215	1227	-6	1	1571	1550	13	2	291	301
7	8	502	523	-1	11	532	541	-5	1	661	646	14	2	1632	1587
9	8	445	493	0	11	517	568	-4	1	1714	1677	15	2	595	554
11	8	840	833	2	11	761	735	-3	1	963	943	16	2	2503	2450
12	8	576	567	3	11	1024	1103	-2	1	759	729	17	2	774	800
13	8	2130	2053	4	11	478	413	-1	1	1997	1990	18	2	1092	1105
15	8	309	302	5	11	609	622	0	1	3056	3098	19	2	751	780
17	8	1222	1153	6	11	732	728	1	1	1394	1373	20	2	382	292
-14	9	203	225	8	11	334	390	2	1	1268	1256	21	2	312	312
-13	9	605	622	10	11	341	371	3	1	1277	1287	22	2	736	734
-12	9	1185	1144	11	11	530	553	4	1	857	818	-21	3	742	785
-11	9	569	613	12	11	593	571	5	1	809	747	-18	3	808	773
-10	9	1060	1069	-8	12	601	575	6	1	1896	1855	-17	3	980	1015
-8	9	364	353	-6	12	358	413	7	1	1441	1491	-16	3	731	767
-6	9	777	823	-3	12	311	346	8	1	2471	2456	-15	3	503	472
-5	9	613	536	0	12	274	313	9	1	1933	1950	-14	3	440	463
-4	9	296	311	2	12	232	199	10	1	370	297	-13	3	952	916
-3	9	826	792	3	12	273	262	11	1	1172	1149	-11	3	508	508
0	9	621	658	6	12	525	520	12	1	275	309	-10	3	1293	1254
2	9	530	532	9	12	394	389	13	1	491	465	-9	3	1736	1781
3	9	465	486	-2	13	278	254	14	1	534	500	-8	3	1288	1308
4	9	1030	1024	-1	13	268	250	15	1	406	425	-7	3	358	320
5	9	1149	1111	0	13	438	448	16	1	279	255	-6	3	644	697
6	9	642	678	1	13	483	479	17	1	1581	1552	-5	3	578	588
7	9	688	673	2	13	180	173	20	1	708	717	-4	3	688	721
9	9	535	479		**L =	-3****		21	1	610	609	-1	3	1654	1689
11	9	674	660	-21	0	353	349	22	1	556	531	0	3	921	868
12	9	1497	1439	-19	0	276	227	-21	2	225	223	1	3	1831	1838
13	9	501	535	-17	0	647	638	-20	2	766	778	2	3	2897	2924
14	9	978	914	-13	0	658	643	-19	2	493	458	4	3	406	462
15	9	307	291	-11	0	802	830	-17	2	801	828	5	3	475	466
16	9	655	612	-9	0	1867	1856	-16	2	1546	1581	6	3	481	431
-13	10	232	248	-7	0	4353	4506	-15	2	290	281	7	3	481	477
-12	10	706	707	-5	0	413	389	-14	2	1407	1507	8	3	414	426
-5	10	1278	1371	-3	0	606	639	-13	2	521	518	9	3	2078	2105
-4	10	2150	2201	-1	0	3109	3166	-12	2	435	448	10	3	2275	2330
-3	10	296	273	1	0	4366	4912	-11	2	486	528	11	3	734	744
-2	10	1305	1247	3	0	236	165	-10	2	574	585	12	3	455	428
-1	10	732	667	7	0	2372	2353	-8	2	498	467	13	3	750	712
1	10	700	637	9	0	910	825	-7	2	273	233	15	3	1879	1825
2	10	501	527	11	0	686	550	-6	2	722	722	16	3	519	522
3	10	351	268	13	0	701	641	-5	2	307	285	17	3	479	495
4	10	1809	1822	15	0	365	399	-4	2	481	464	18	3	1354	1268
5	10	819	815	17	0	692	724	-3	2	450	426	19	3	476	472
6	10	1688	1691	19	0	326	273	-2	2	1161	1160	20	3	453	479
7	10	426	437	21	0	417	390	-1	2	2624	2606	21	3	272	247
8	10	352	413	-19	1	278	277	0	2	1031	987	22	3	678	619
10	10	481	534	-18	1	355	317	1	2	1737	1672	-18	4	751	750

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-3****													
-15	4	546	508	10	5	627	617	8	7	551	589	-3	10	363	418
-14	4	606	583	11	5	1252	1265	9	7	663	639	-2	10	572	648
-13	4	859	840	12	5	346	399	11	7	539	498	-1	10	397	300
-11	4	1300	1322	14	5	305	245	12	7	1016	978	2	10	308	351
-10	4	1375	1420	15	5	684	620	13	7	267	39	3	10	698	676
-9	4	1408	1443	16	5	590	562	14	7	800	752	5	10	1467	1408
-8	4	1605	1607	18	5	534	469	15	7	387	360	6	10	1150	1216
-7	4	1804	1754	19	5	406	431	16	7	742	692	11	10	617	587
-6	4	1060	1041	20	5	969	908	18	7	418	430	12	10	373	343
-5	4	769	775	-19	6	388	408	19	7	256	256	13	10	1160	1170
-4	4	615	593	-18	6	296	316	-17	8	227	232	14	10	423	424
-3	4	1843	1865	-17	6	518	519	-16	8	635	674	-11	11	300	282
-2	4	2769	2831	-14	6	439	415	-14	8	243	272	-10	11	208	272
-1	4	1672	1629	-13	6	1062	1044	-12	8	1773	1818	-7	11	491	511
0	4	759	703	-12	6	420	443	-11	8	330	279	-6	11	951	1039
1	4	2204	2152	-11	6	588	597	-10	8	828	888	-5	11	537	596
2	4	2712	2707	-9	6	418	434	-9	8	426	379	-3	11	1288	1398
3	4	2001	1962	-8	6	613	636	-8	8	357	284	-2	11	856	869
4	4	1239	1174	-5	6	466	438	-7	8	528	565	-1	11	571	589
6	4	529	569	-4	6	450	451	-5	8	618	643	0	11	884	943
7	4	451	430	-2	6	820	894	-4	8	1523	1541	1	11	490	447
9	4	942	911	-1	6	305	264	-2	8	245	238	2	11	659	652
10	4	448	396	0	6	1253	1210	4	8	1664	1558	4	11	458	370
11	4	250	209	1	6	446	439	6	8	687	636	5	11	1149	1114
12	4	385	404	2	6	304	303	7	8	273	205	6	11	861	898
15	4	389	386	3	6	851	831	10	8	402	395	7	11	978	965
16	4	509	460	5	6	2023	2005	12	8	512	541	9	11	389	417
17	4	338	284	6	6	1850	1826	16	8	448	444	11	11	422	416
18	4	724	679	7	6	762	750	-15	9	823	817	12	11	345	322
19	4	255	154	8	6	599	568	-13	9	495	508	-8	12	568	530
20	4	402	422	10	6	308	278	-12	9	624	621	-7	12	435	465
-20	5	229	286	11	6	916	925	-11	9	993	1029	-6	12	268	292
-18	5	558	575	12	6	369	363	-10	9	451	428	-5	12	726	743
-16	5	847	863	13	6	1198	1154	-6	9	396	403	-4	12	304	296
-15	5	458	439	14	6	1174	1178	-5	9	758	837	-3	12	471	520
-14	5	1103	1116	15	6	298	352	-4	9	644	704	-2	12	940	1016
-13	5	257	160	19	6	650	646	-3	9	959	1008	-1	12	776	841
-12	5	341	337	20	6	413	373	1	9	330	324	1	12	513	540
-10	5	483	517	-18	7	833	849	2	9	350	351	2	12	626	625
-9	5	821	822	-13	7	372	424	3	9	442	361	3	12	783	807
-8	5	735	707	-12	7	545	559	4	9	574	630	4	12	419	406
-7	5	867	895	-11	7	908	893	5	9	564	576	6	12	235	194
-6	5	923	989	-10	7	414	413	6	9	602	613	7	12	539	563
-5	5	1103	1078	-8	7	359	296	10	9	436	401	8	12	429	435
-3	5	1408	1487	-7	7	259	240	11	9	335	305	9	12	301	245
-2	5	1779	1717	-6	7	482	522	12	9	1291	1265	10	12	258	262
-1	5	1237	1253	-5	7	1817	1913	13	9	311	234	-2	13	321	352
0	5	776	756	-4	7	782	785	14	9	415	441	-1	13	312	321
1	5	691	697	-3	7	1202	1204	16	9	453	449	1	13	345	362
3	5	645	621	-2	7	830	838	-14	10	308	294	1	13	446	455
4	5	899	856	-1	7	352	432	-13	10	462	488	2	13	542	560
5	5	1837	1726	2	7	289	280	-11	10	888	914	3	13	220	272
6	5	1088	1100	3	7	1583	1545	-10	10	224	242	4	13		
7	5	1479	1457	4	7	739	700	-9	10	512	530	**L =	-2****		
8	5	561	548	5	7	745	693	-8	10	325	340	-22	0	282	343
9	5	313	298	6	7	726	685	-8	10	325	267	-20	0	336	312
				7	7	634	621	-7	10	325	267	-16	0	685	677
								-6	10	366	378	-14	0	648	610

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
-12	0	746	681	-13	2	755	761	11	3	982	939	-2	5	470	463
-10	0	871	875	-11	2	815	792	12	3	769	706	-1	5	459	443
-8	0	234	192	-10	2	1791	1850	13	3	1382	1372	0	5	572	529
-6	0	892	865	-9	2	1976	1985	15	3	1406	1338	1	5	1041	960
-4	0	907	870	-8	2	477	473	16	3	366	425	2	5	2454	2465
-2	0	870	792	-7	2	2060	2142	17	3	894	945	3	5	3071	3086
0	0	4956	5833	-6	2	2193	2243	18	3	1156	1120	4	5	1717	1682
2	0	2674	2703	-5	2	231	280	19	3	977	942	5	5	577	512
4	0	1843	1809	-4	2	299	214	21	3	284	264	6	5	557	552
6	0	1074	1066	-3	2	925	915	22	3	428	413	7	5	950	937
8	0	4531	4592	-2	2	218	216	-21	4	489	495	8	5	259	199
10	0	2764	2633	-1	2	2636	2637	-20	4	349	374	9	5	348	297
12	0	398	459	0	2	485	443	-19	4	771	791	10	5	1055	1058
14	0	912	890	1	2	2932	2948	-17	4	637	673	11	5	1252	1269
16	0	969	965	2	2	264	194	-16	4	628	589	14	5	966	925
18	0	734	736	3	2	461	480	-14	4	650	700	15	5	1057	971
20	0	331	326	4	2	996	976	-13	4	398	387	16	5	431	418
-21	1	818	855	5	2	714	643	-11	4	650	631	18	5	347	289
-20	1	484	478	6	2	206	231	-10	4	394	365	19	5	394	388
-18	1	409	411	7	2	244	215	-7	4	761	808	21	5	438	447
-17	1	974	1025	10	2	641	573	-6	4	910	878	-19	6	719	727
-16	1	1320	1289	12	2	402	363	-5	4	352	316	-18	6	227	222
-15	1	319	294	15	2	846	834	-2	4	1505	1442	-14	6	380	381
-12	1	345	362	17	2	1062	1045	-1	4	1871	1843	-13	6	1017	1093
-11	1	456	395	18	2	785	802	1	4	1535	1513	-12	6	965	985
-10	1	570	571	21	2	849	842	2	4	1517	1445	-11	6	379	455
-8	1	3564	3652	22	2	319	321	3	4	2566	2506	-10	6	856	889
-7	1	1631	1660	-21	3	297	320	4	4	2038	1993	-9	6	446	475
-6	1	2115	2115	-20	3	455	482	5	4	289	275	-8	6	640	667
-5	1	680	643	-19	3	537	568	6	4	1965	1989	-7	6	381	372
-4	1	938	903	-18	3	606	584	7	4	976	984	-6	6	663	704
-3	1	1361	1293	-17	3	581	556	8	4	858	930	-5	6	1927	1961
-2	1	753	715	-16	3	653	640	9	4	1939	1982	-4	6	2558	2625
-1	1	1551	1538	-15	3	1391	1394	10	4	1391	1398	-2	6	1607	1696
0	1	2041	2043	-14	3	1302	1311	11	4	1797	1788	-1	6	731	712
1	1	2347	2409	-13	3	446	474	12	4	682	691	1	6	385	330
2	1	1210	1228	-12	3	921	962	14	4	1439	1405	2	6	1185	1205
3	1	315	261	-11	3	884	854	15	4	753	783	3	6	253	267
4	1	1818	1724	-10	3	779	817	16	4	444	449	4	6	1403	1423
5	1	1603	1516	-9	3	2034	2056	17	4	510	485	5	6	559	502
6	1	2201	2150	-8	3	1281	1301	19	4	1051	1079	8	6	443	451
7	1	1648	1576	-7	3	1517	1493	21	4	245	253	11	6	512	525
8	1	1113	1092	-6	3	644	607	-20	5	504	564	13	6	324	295
9	1	1856	1834	-4	3	1668	1667	-19	5	492	497	14	6	627	618
11	1	562	597	-3	3	844	831	-18	5	653	641	16	6	317	273
15	1	906	911	-2	3	2183	2260	-17	5	292	311	18	6	473	506
16	1	821	808	-1	3	2207	2236	-14	5	377	370	19	6	775	731
17	1	818	846	0	3	831	813	-13	5	385	364	20	6	773	740
18	1	628	579	1	3	578	584	-12	5	531	552	-16	7	549	604
19	1	297	217	2	3	349	366	-11	5	458	420	-14	7	472	484
-20	2	500	497	4	3	596	630	-10	5	1236	1213	-13	7	968	989
-19	2	690	686	5	3	1068	1039	-9	5	1190	1247	-12	7	607	651
-18	2	1271	1248	6	3	1177	1167	-7	5	356	364	-11	7	1398	1424
-17	2	1032	1027	7	3	1576	1518	-6	5	1564	1608	-10	7	281	185
-15	2	1832	1870	8	3	293	287	-5	5	1854	1926	-9	7	318	283
-14	2	1172	1176	9	3	1601	1617	-4	5	452	500	-8	7	583	568
				10	3	2169	2178	-3	5	1152	1168	-6	7	846	861

Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
**L = -2****				-3	9	827	826	-1	12	520	496	-1	1	2423	2473
-5	7	311	339	0	9	318	369	1	12	357	385	0	1	1619	1667
-3	7	1553	1543	3	9	409	421	2	12	802	806	1	1	2626	2805
-2	7	615	584	4	9	1978	2001	3	12	721	781	2	1	177	153
0	7	411	418	5	9	975	1036	4	12	406	398	3	1	585	591
1	7	656	621	6	9	608	615	5	12	343	366	4	1	1283	1275
2	7	261	216	7	9	274	326	6	12	949	1000	5	1	816	781
3	7	572	544	12	9	1567	1539	8	12	426	442	6	1	3298	3259
4	7	1626	1680	14	9	474	416	9	12	613	625	7	1	889	873
5	7	1394	1436	15	9	460	423	10	12	704	711	8	1	301	280
6	7	907	845	16	9	900	886	-4	13	303	367	9	1	1570	1548
7	7	428	358	-14	10	226	206	-3	13	523	506	10	1	550	549
9	7	985	953	-13	10	643	650	-2	13	552	572	12	1	670	649
10	7	757	665	-12	10	1187	1205	-1	13	293	286	15	1	382	320
12	7	1469	1450	-11	10	270	200	0	13	259	330	16	1	1127	1138
13	7	379	239	-10	10	494	439	1	13	206	182	17	1	1136	1076
15	7	556	531	-7	10	577	611	2	13	313	302	18	1	904	821
16	7	285	327	-6	10	679	735	3	13	326	342	20	1	753	715
17	7	367	365	-5	10	1075	1073	5	13	327	360	21	1	569	538
18	7	599	534	-4	10	1916	1985	**L = -1****				22	1	373	389
19	7	819	721	-2	10	1014	1035	-19	0	503	520	-22	2	608	655
-17	8	656	672	-1	10	393	403	-17	0	1523	1536	-20	2	361	336
-16	8	216	182	1	10	773	831	-15	0	510	545	-19	2	370	367
-13	8	538	528	2	10	579	630	-13	0	279	333	-16	2	662	642
-11	8	420	381	3	10	344	363	-11	0	1871	1840	-14	2	433	514
-9	8	416	358	4	10	722	703	-9	0	2477	2411	-13	2	346	317
-7	8	492	586	5	10	737	751	-7	0	3459	3579	-12	2	333	288
-6	8	389	432	6	10	662	707	-5	0	876	848	-11	2	402	356
-5	8	253	311	10	10	232	243	-3	0	839	791	-9	2	1184	1136
-4	8	284	301	12	10	373	329	-1	0	2434	2460	-8	2	1991	1947
-3	8	623	597	15	10	374	326	1	0	2003	1995	-7	2	2238	2267
-1	8	755	819	-12	11	292	304	5	0	275	240	-6	2	501	476
0	8	274	259	-11	11	484	481	7	0	732	723	-5	2	649	644
1	8	427	386	-10	11	645	662	9	0	1200	1162	-4	2	246	230
2	8	359	315	-9	11	263	260	11	0	1269	1213	-3	2	1408	1381
3	8	852	815	-6	11	809	758	13	0	323	278	-2	2	237	254
4	8	425	450	-5	11	774	815	15	0	608	554	-1	2	819	834
5	8	2318	2266	-4	11	409	356	17	0	2433	2359	0	2	309	319
6	8	612	659	-3	11	547	547	19	0	427	383	2	2	638	606
7	8	353	306	-2	11	612	606	-21	1	320	283	3	2	345	351
8	8	354	358	0	11	295	284	-20	1	427	385	4	2	1566	1503
11	8	1719	1686	1	11	699	691	-18	1	269	267	6	2	1008	965
12	8	450	398	2	11	1221	1254	-17	1	272	270	7	2	2888	2931
13	8	2315	2153	3	11	1063	1078	-16	1	1058	1094	8	2	2607	2636
15	8	503	510	4	11	975	991	-15	1	658	658	9	2	945	962
16	8	247	256	5	11	263	218	-13	1	624	598	11	2	935	948
17	8	812	786	6	11	246	186	-12	1	820	831	12	2	1748	1718
-15	9	318	304	7	11	534	540	-11	1	433	386	13	2	255	255
-14	9	461	478	9	11	297	280	-10	1	1012	1001	14	2	1300	1318
-13	9	866	880	10	11	382	365	-9	1	1037	1051	15	2	608	601
-12	9	311	344	11	11	333	325	-8	1	1367	1427	16	2	1296	1282
-11	9	1126	1164	12	11	337	307	-7	1	800	768	17	2	401	418
-10	9	850	923	13	11	353	358	-6	1	610	601	18	2	611	526
-9	9	280	291	-7	12	197	217	-5	1	2223	2123	19	2	475	394
-6	9	474	514	-6	12	272	286	-4	1	731	662	20	2	382	372
-5	9	651	704	-3	12	276	241	-3	1	235	183	21	2	320	286
-4	9	507	508	-2	12	492	497	-2	1	1246	1238	-21	3	438	468



Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
	**L =	-1***													
-20	3	283	327	1	4	693	704	-6	6	1585	1641	-4	8	1389	1418
-19	3	646	674	2	4	725	717	-5	6	1077	1129	-2	8	260	277
-18	3	354	317	3	4	1076	1046	-4	6	503	537	-1	8	765	790
-17	3	1190	1265	4	4	419	391	-3	6	2937	3077	0	8	302	303
-16	3	680	722	6	4	446	486	-2	6	916	925	7	8	313	293
-15	3	259	268	8	4	342	301	-1	6	626	639	8	8	408	345
-14	3	1444	1451	9	4	491	448	1	6	993	1020	11	8	353	314
-11	3	908	925	10	4	1350	1338	2	6	1493	1572	12	8	1725	1678
-9	3	616	668	11	4	994	957	3	6	3016	3005	14	8	611	580
-8	3	865	896	12	4	231	124	4	6	877	766	16	8	1132	1075
-7	3	1271	1295	13	4	509	468	5	6	2690	2602	17	8	250	220
-6	3	1923	1929	15	4	982	1001	6	6	1769	1735	18	8	863	844
-5	3	1224	1230	18	4	1628	1595	7	6	947	912	-16	9	297	340
-4	3	1445	1466	20	4	566	523	8	6	990	979	-15	9	686	742
-3	3	276	267	21	4	311	322	11	6	1216	1183	-14	9	447	462
-2	3	380	410	-19	5	528	526	13	6	1178	1152	-13	9	1202	1317
-1	3	642	619	-18	5	249	304	14	6	1051	1018	-12	9	354	345
0	3	1054	1026	-16	5	444	488	17	6	278	243	-11	9	1236	1271
1	3	1817	1758	-15	5	868	870	-19	7	609	641	-7	9	292	286
2	3	3857	3929	-14	5	1150	1190	-18	7	525	568	-6	9	666	735
3	3	1398	1361	-12	5	352	278	-17	7	723	700	-5	9	1052	1097
4	3	635	612	-11	5	1108	1105	-15	7	385	341	-4	9	1226	1311
5	3	374	360	-10	5	1168	1224	-14	7	335	313	-3	9	721	718
6	3	1356	1414	-9	5	1153	1178	-13	7	1428	1505	-2	9	305	366
7	3	1912	1872	-8	5	310	263	-12	7	436	447	2	9	331	260
8	3	717	710	-6	5	468	468	-11	7	998	1061	4	9	1411	1341
9	3	864	859	-5	5	361	401	-10	7	410	433	5	9	615	547
10	3	1810	1772	-4	5	1137	1143	-9	7	1024	1065	6	9	751	698
12	3	639	574	-3	5	2026	2099	-8	7	623	639	9	9	283	200
13	3	1209	1164	-2	5	2343	2447	-6	7	399	347	10	9	568	578
14	3	1664	1625	-1	5	1726	1700	-5	7	1965	2008	11	9	525	473
15	3	1398	1381	0	5	256	244	-4	7	1715	1831	12	9	1251	1247
16	3	1321	1285	1	5	1032	983	-3	7	470	465	13	9	945	903
17	3	360	392	2	5	1748	1723	-1	7	423	404	14	9	648	625
18	3	689	632	3	5	1864	1801	1	7	563	507	-12	10	228	218
19	3	994	946	4	5	719	674	3	7	1104	1123	-10	10	413	429
20	3	422	424	5	5	602	565	4	7	2005	1980	-6	10	517	481
22	3	623	575	6	5	812	785	5	7	1360	1396	-5	10	1098	1180
-21	4	641	638	7	5	366	412	6	7	1035	976	-4	10	369	319
-20	4	385	385	8	5	363	411	8	7	824	765	-3	10	1173	1205
-18	4	1254	1326	9	5	756	750	9	7	1028	987	-2	10	951	954
-15	4	1130	1149	10	5	1465	1476	10	7	618	561	0	10	472	466
-14	4	698	703	11	5	1224	1207	11	7	502	446	2	10	850	862
-13	4	971	1008	12	5	508	459	12	7	1362	1331	3	10	1498	1494
-11	4	1888	1932	14	5	493	401	13	7	1134	1138	5	10	1803	1790
-10	4	2320	2340	15	5	432	388	14	7	558	578	6	10	1329	1358
-9	4	1414	1420	18	5	244	169	17	7	450	457	11	10	654	683
-8	4	736	744	19	5	930	883	19	7	382	311	13	10	894	888
-7	4	1119	1138	20	5	333	326	-16	8	1023	1046	14	10	229	240
-6	4	1032	1102	21	5	232	251	-15	8	245	264	-12	11	295	309
-5	4	496	519	-19	6	240	259	-14	8	440	463	-11	11	752	770
-4	4	268	275	-17	6	422	410	-12	8	2440	2604	-10	11	496	528
-3	4	1853	1943	-14	6	476	517	-11	8	502	441	-8	11	454	491
-2	4	1329	1345	-12	6	431	449	-10	8	829	945	-6	11	500	492
-1	4	1382	1340	-11	6	288	289	-8	8	557	685	-4	11	670	689
0	4	758	761	-9	6	231	187	-7	8	508	555	-3	11	1436	1409
				-8	6	735	728	-5	8	300	244	-2	11	837	834



Table 44. Continued

H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL	H	K	FOBS	FCAL
**L = -1****				-9	1	650	660	-11	4	1033	1056	-11	7	766	745
-1	11	871	883	-8	1	2502	2507	-10	4	1226	1296	-4	7	1699	1791
0	11	390	407	-7	1	1488	1492	-9	4	1750	1842	-3	7	678	706
2	11	248	213	-6	1	2861	2809	-8	4	898	880	-2	7	693	727
3	11	783	778	-5	1	1140	1075	-7	4	248	270	-18	8	296	337
4	11	1124	1161	-4	1	1177	1149	-6	4	1419	1546	-13	8	867	877
5	11	774	770	-3	1	727	751	-5	4	353	400	-11	8	1085	1096
6	11	237	268	-1	1	2670	2849	-4	4	1644	1655	-7	8	558	560
7	11	506	528	-22	2	281	289	-3	4	725	713	-5	8	1541	1578
8	11	278	251	-21	2	815	820	-2	4	2308	2333	-3	8	1016	1070
10	11	484	467	-19	2	385	425	-1	4	3044	3114	-2	8	593	587
11	11	838	835	-18	2	1395	1421	0	4	833	744	-1	8	748	701
12	11	599	553	-17	2	1520	1512	-20	5	343	342	-16	9	501	601
-9	12	468	487	-16	2	269	281	-19	5	522	514	-15	9	296	307
-8	12	387	425	-15	2	1970	2049	-17	5	583	588	-13	9	645	653
-7	12	441	518	-14	2	984	982	-16	5	329	340	-12	9	521	541
-5	12	638	658	-13	2	1145	1203	-15	5	669	618	-11	9	852	837
-3	12	411	438	-12	2	645	617	-14	5	1177	1179	-7	9	313	288
-2	12	523	525	-11	2	727	780	-13	5	263	316	-4	9	1252	1296
-1	12	416	383	-10	2	1019	1088	-9	5	612	598	-3	9	517	618
5	12	251	224	-9	2	1237	1258	-7	5	1087	1131	-15	10	381	333
8	12	215	219	-8	2	873	852	-6	5	1281	1408	-14	10	316	334
10	12	348	278	-7	2	1057	1089	-5	5	1294	1400	-13	10	265	271
0	13	189	189	-6	2	1204	1216	-3	5	1699	1716	-12	10	954	952
1	13	274	268	-5	2	330	264	-2	5	2104	2166	-10	10	341	372
2	13	339	368	-4	2	251	283	-1	5	559	507	-8	10	286	349
3	13	346	326	-2	2	228	223	-20	6	794	845	-7	10	478	500
4	13	204	215	0	2	200	142	-19	6	906	951	-6	10	384	413
5	13	226	209	-22	3	583	652	-18	6	326	424	-4	10	826	884
**L = 0****				-20	3	387	457	-17	6	329	316	-2	10	297	411
-22	0	318	383	-19	3	837	818	-15	6	546	581	-7	11	499	510
-18	0	490	459	-17	3	1009	1009	-14	6	794	801	-6	11	775	846
-16	0	628	623	-16	3	995	1004	-13	6	1082	1116	-5	11	849	879
-14	0	633	607	-15	3	519	540	-12	6	1090	1110	-4	11	996	1051
-12	0	297	286	-14	3	1456	1474	-10	6	709	756	-2	11	658	666
-10	0	1314	1282	-13	3	488	501	-9	6	340	423	-1	11	596	598
-8	0	3276	3398	-11	3	1102	1121	-8	6	419	373	-9	12	608	596
-6	0	838	820	-10	3	1801	1832	-6	6	1019	1104	-8	12	284	298
-4	0	1348	1307	-9	3	1860	1933	-5	6	574	617	-7	12	249	237
-2	0	2461	2457	-8	3	655	640	-4	6	1211	1234	-6	12	894	925
-22	1	430	390	-7	3	504	508	-3	6	231	287	-5	12	202	173
-21	1	643	668	-5	3	466	448	-2	6	339	375	-3	12	663	680
-20	1	382	401	-4	3	247	252	-1	6	251	203	-2	12	941	989
-18	1	588	623	-3	3	1830	1832	0	6	340	361	-1	12	589	600
-17	1	373	338	-2	3	2192	2205	-19	7	528	548	0	12	282	315
-16	1	1866	1907	-1	3	1371	1303	-18	7	488	522	-5	13	345	355
-15	1	244	134	-18	4	263	142	-17	7	372	412	-3	13	605	611
-12	1	370	368	-15	4	351	353	-14	7	417	398	-2	13	540	550
-11	1	1479	1469	-14	4	379	460	-13	7	929	973	-1	13	189	223
-10	1	470	443	-12	4	343	303	-12	7	902	930				

Table 45. 10\*(Fobs vs. Fcal) For [Rh2C12(CO)(C2S4)(DPM)2].

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	0****		15	0	605	576	20	16	651	735	25	2	1297	1413
0	2	9929	8960	15	1	397	286	21	-1	2267	1844	25	6	387	303
0	4	1412	580	15	2	556	681	21	0	1447	1662	25	7	718	693
0	6	1254	929	15	3	614	617	21	1	2013	1961	25	8	903	803
0	8	676	601	15	5	498	523	21	2	1578	1629	25	9	1202	1133
0	10	1173	1237	15	6	479	530	21	3	956	1035	25	10	395	282
0	12	833	896	15	8	1178	1336	21	5	422	590	25	11	443	194
0	14	1256	1166	15	10	682	818	21	6	584	541	25	12	466	434
0	16	2025	1819	16	0	1048	1011	21	7	1633	1574	25	13	471	283
0	18	1534	1527	16	1	754	836	21	9	1077	957	25	17	738	733
0	20	632	679	16	2	523	519	21	10	1263	1288	26	0	769	275
8	0	999	1079	16	7	509	568	21	11	452	396	26	1	2728	3213
8	1	439	476	16	8	856	819	21	12	1743	1711	26	2	769	891
8	4	362	235	17	-1	2811	2957	21	14	711	853	26	3	690	1144
8	6	357	238	17	1	1173	1432	21	16	1034	932	26	4	663	563
9	-1	1208	1215	17	2	487	522	21	18	776	727	26	5	1257	1421
9	1	606	677	17	3	616	775	22	0	5685	5922	26	7	2548	2312
9	5	467	446	17	4	385	410	22	2	747	1043	26	9	778	985
10	0	1185	1158	17	6	1266	1438	22	5	1256	1304	26	11	458	413
10	2	817	818	17	8	1603	1682	22	6	553	694	26	13	486	426
10	5	430	492	17	9	535	571	22	7	1867	1799	26	16	743	634
10	7	525	628	17	12	539	681	22	8	388	280	26	17	541	506
10	8	461	558	17	13	650	662	22	9	3042	2882	27	-1	4544	4476
10	9	488	560	18	0	2420	2790	22	10	424	373	27	0	392	894
10	10	397	476	18	2	1512	1907	22	11	469	545	27	1	1951	1984
11	-1	1970	1946	18	4	714	864	22	16	742	670	27	2	1287	1382
11	1	1172	1162	18	8	477	308	22	17	590	478	27	3	260	542
11	3	999	995	18	13	623	526	22	18	475	587	27	4	289	868
11	5	955	1031	18	14	1198	1254	23	-1	4059	4089	27	5	1621	1531
11	8	964	945	18	16	754	572	23	0	1771	2014	27	6	2590	2347
12	1	848	810	19	-1	4064	4227	23	1	1526	1805	27	8	3395	3177
12	4	562	484	19	0	620	704	23	2	398	449	27	9	737	660
12	5	559	686	19	1	468	620	23	3	1108	1342	27	10	2290	2358
12	6	1008	1126	19	3	1132	1192	23	4	1346	1515	27	11	620	571
12	7	1700	1826	19	4	510	479	23	5	1931	1815	27	13	796	808
12	8	808	979	19	5	778	940	23	7	1214	1360	27	15	642	471
12	9	1307	1340	19	6	1064	1024	23	9	1937	1866	28	1	970	1185
13	-1	1482	1557	19	7	1396	1250	23	10	555	540	28	2	926	551
13	1	707	749	19	8	995	916	24	0	4748	5254	28	3	1002	1177
13	2	479	594	19	10	1336	1219	24	1	1352	959	28	4	1679	1538
13	5	693	693	19	12	981	953	24	2	1761	996	28	5	1131	1192
13	6	461	615	19	13	829	824	24	3	690	701	28	6	911	1040
13	8	723	873	19	15	949	822	24	4	496	528	28	7	842	528
13	10	747	800	19	16	690	702	24	5	822	908	28	8	2390	2175
13	12	415	529	19	17	603	566	24	7	341	271	28	9	551	410
13	13	452	537	20	0	2576	2669	24	8	911	713	28	10	1001	893
14	0	1325	1381	20	1	1485	1326	24	9	882	884	28	11	780	771
14	1	853	795	20	3	1702	1811	24	10	748	794	28	12	626	620
14	2	512	610	20	4	592	611	24	11	910	951	28	13	1086	1016
14	3	600	568	20	5	1024	1127	24	12	446	325	28	14	1406	1314
14	5	427	625	20	7	3831	3730	24	13	488	501	28	15	508	368
14	6	554	534	20	9	3894	4015	24	14	638	558				
14	8	599	588	20	11	1720	1676	24	16	1010	919		**H =	1****	
14	9	750	802	20	12	601	428	24	18	550	416	0	0	933	1876
14	11	653	766	20	13	646	673	25	-1	442	952	0	2	226	146
14	13	424	490	20	14	982	1059	25	0	595	1036	0	4	1987	1946
15	-1	606	218	20	15	742	836	25	0	1299	1329	0	6	5994	5318
									1			0	8	7370	7001

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	1****		17	-1	600	927	22	6	2546	2609	26	11	463	213
0	10	3815	3776	17	4	402	611	22	7	496	332	26	12	899	852
0	12	1221	1283	17	5	666	700	22	8	3625	3766	26	13	518	357
0	16	876	841	17	7	1200	1236	22	10	1223	1333	26	14	515	469
0	18	493	688	17	14	624	632	22	11	530	555	26	18	451	443
7	0	927	971	18	-1	1365	1411	22	13	559	498	27	0	4949	5715
8	-1	404	390	18	0	482	583	22	15	991	889	27	2	1424	1435
8	3	515	437	18	3	725	776	22	16	591	463	27	3	1874	1867
8	5	377	412	18	4	968	1127	22	17	1025	1019	27	4	1647	1268
8	6	518	580	18	6	2452	2853	22	18	471	423	27	5	2258	2140
9	3	363	382	18	8	2286	2496	23	-1	3766	4491	27	7	2286	2216
9	5	677	753	18	9	563	522	23	0	516	800	27	8	1140	1066
9	7	683	791	18	15	707	689	23	1	1778	1888	27	9	1200	1157
10	-1	822	936	19	-1	924	1076	23	2	1467	1394	27	13	474	274
10	4	605	625	19	0	1615	1618	23	3	802	728	27	14	1214	1065
10	6	1155	1254	19	1	1391	1273	23	7	635	546	27	15	634	594
10	7	577	557	19	2	497	616	23	9	1315	1293	27	16	1565	1584
10	8	886	960	19	3	675	698	23	10	587	537	27	17	446	489
11	5	619	564	19	4	664	731	23	11	447	522	27	18	900	979
11	6	421	447	19	5	2646	2830	23	15	950	904	28	-1	215	458
11	7	1047	1102	19	6	1361	1513	23	16	557	383	28	0	2546	2851
11	9	1058	1184	19	7	2881	3046	23	17	606	488	28	1	1539	1304
11	11	750	849	19	8	839	852	24	-1	1442	1558	28	2	1362	1685
12	-1	2129	2058	19	9	593	673	24	0	1095	1230	28	3	1814	1966
12	0	656	501	19	11	997	1012	24	1	351	241	28	4	618	664
12	1	1221	1167	19	13	677	740	24	2	941	1487	28	6	2150	1974
12	4	727	742	19	15	559	701	24	4	849	844	28	7	905	747
12	7	408	371	20	-1	5604	6417	24	5	1205	1263	28	8	934	817
12	9	608	623	20	0	793	1101	24	6	1991	1940	28	9	539	498
12	10	766	784	20	1	3672	4240	24	7	473	505	28	10	2065	2097
12	12	781	829	20	3	1452	1612	24	8	2324	2454	28	11	820	737
13	0	588	641	20	5	778	848	24	9	525	416	28	12	1123	1091
13	1	1031	1123	20	6	1825	1558	24	10	421	379	28	13	955	931
13	2	641	666	20	7	606	749	24	11	545	444	28	14	561	605
13	3	564	655	20	8	487	548	25	-1	1332	1870	28	15	591	535
13	4	503	503	20	13	875	701	25	0	346	918	28	16	1036	987
13	5	703	711	20	15	711	717	25	1	1067	963	28	18	474	477
13	6	587	513	20	17	847	792	25	2	1832	1857	28	19	512	568
13	7	1330	1358	21	0	943	946	25	3	1207	1518	**H = 2****			
13	9	767	896	21	2	1995	2374	25	4	691	561	0	0	9509	9265
13	10	390	367	21	3	1409	1644	25	5	823	748	0	2	1623	1590
14	-1	693	813	21	4	435	661	25	7	1611	1638	0	4	3058	2457
14	0	604	622	21	5	2115	2195	25	9	923	993	0	8	987	970
14	5	865	1005	21	6	1634	1652	25	11	438	445	0	12	877	658
14	6	483	569	21	7	1248	1248	25	12	536	577	0	14	1709	1617
14	7	880	793	21	8	457	400	25	14	775	668	0	16	1882	1903
14	8	700	773	21	9	771	936	25	15	971	1006	0	18	1368	1611
14	9	504	398	21	11	741	730	25	16	522	641	7	2	381	315
15	0	1057	1193	21	12	757	727	26	-1	1343	1513	8	-2	832	905
15	1	395	482	21	13	535	560	26	0	608	991	8	-1	561	441
16	-1	1165	1266	21	14	971	939	26	1	847	516	9	-2	610	535
16	0	515	451	21	15	558	658	26	2	798	771	9	-1	719	721
16	4	616	601	22	-1	5309	5923	26	3	2578	1903	9	6	357	386
16	6	487	537	22	1	1539	2034	26	4	856	784	10	-2	1531	1557
16	7	473	691	22	2	749	1091	26	5	1727	1914	10	0	664	630
16	13	687	784	22	3	383	67	26	6	1572	1564	10	3	451	343
16	15	739	715	22	4	655	551	26	9	666	541	10	5	1012	1087

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	2****		18	2	1025	1072	22	7	2802	2930	27	5	374	344
10	7	677	791	18	3	695	672	22	9	762	801	27	6	5017	5062
10	8	438	349	18	5	859	860	22	14	1063	991	27	7	884	1010
11	-2	724	765	18	6	813	899	22	16	905	938	27	8	2194	2032
11	-1	927	876	18	8	940	987	23	-2	468	304	27	11	1224	1270
11	1	512	529	18	9	772	935	23	-1	2716	2611	27	13	999	1064
11	3	829	851	18	12	1163	1188	23	0	763	656	27	15	680	670
11	4	611	669	18	14	938	941	23	1	2333	2721	28	-2	341	331
11	5	651	644	18	16	583	565	23	2	636	516	28	-1	2478	2370
11	6	924	1073	19	-2	559	418	23	4	924	979	28	0	1081	1057
11	8	387	523	19	-1	1169	1261	23	6	963	1034	28	1	397	493
11	9	373	174	19	1	845	973	23	8	706	683	28	2	2512	3105
12	-2	1048	937	19	3	903	1020	23	9	779	764	28	3	573	521
12	4	529	594	19	4	680	734	23	13	773	767	28	4	2845	2664
12	5	1341	1423	19	5	1063	1174	24	-2	1443	1486	28	5	2353	2323
12	7	1511	1793	19	6	940	1117	24	-1	700	802	28	6	1246	1201
12	9	523	692	19	8	1189	1246	24	0	1844	1645	28	7	534	462
12	10	471	336	19	10	970	938	24	2	561	187	28	9	1155	1131
13	-1	416	441	19	11	853	838	24	4	396	440	28	10	850	699
13	0	443	368	19	13	1291	1327	24	5	519	515	28	11	927	916
13	1	533	418	19	14	576	648	24	7	673	684	28	12	1043	1005
13	3	428	528	19	15	939	1057	24	8	476	367	28	13	954	1045
13	4	823	863	20	-2	2575	2964	24	9	1047	1046	28	14	606	544
13	6	1291	1428	20	-1	568	856	24	14	580	629	28	15	573	462
13	8	619	840	20	0	825	1201	24	16	571	533	28	18	852	1101
13	10	637	716	20	1	2016	2413	25	-2	1174	1251		**H =	3****	
13	11	501	531	20	3	2278	2562	25	-1	790	1113	0	-2	619	704
14	-2	1090	1201	20	4	855	750	25	0	1250	1903	0	0	2023	2165
14	3	505	725	20	5	4312	4933	25	1	1350	1138	0	2	6723	6163
14	5	682	597	20	6	559	740	25	3	961	1121	0	4	7582	7479
14	7	530	632	20	7	4408	4841	25	4	1015	1035	0	6	9146	8846
14	9	521	451	20	9	1804	1881	25	5	661	600	0	8	4937	4818
14	10	476	446	20	10	720	654	25	6	1595	1735	0	10	362	344
14	12	422	495	20	12	689	808	25	7	608	470	0	12	686	762
14	13	487	561	20	14	606	495	25	14	672	742	0	14	1037	969
15	-2	778	953	20	15	822	993	25	15	1092	1119	0	16	839	972
15	-1	467	407	20	16	675	455	25	17	619	687	7	-2	919	944
15	0	714	873	21	-2	3139	3290	26	-2	722	1030	8	4	436	548
15	5	424	426	21	-1	2229	2744	26	-1	669	997	9	-3	463	503
15	6	1577	1807	21	0	1425	1351	26	0	831	909	9	-1	456	471
15	8	1058	1159	21	1	440	668	26	1	3761	3638	9	3	503	590
15	14	522	499	21	2	594	792	26	3	1776	1356	9	5	899	1005
16	-2	1536	1751	21	4	748	742	26	5	3315	3457	10	-3	547	593
16	-1	1093	1106	21	5	1113	1108	26	6	462	588	10	2	651	613
16	0	1507	1681	21	6	710	796	26	7	2080	2096	10	4	1165	1174
16	3	485	475	21	7	1054	1169	26	8	373	280	10	6	964	994
16	5	1114	1225	21	8	995	1009	26	9	425	282	10	8	426	469
16	7	756	777	21	10	1392	1489	26	11	547	501	11	-2	620	675
16	13	458	407	21	12	876	995	26	12	488	338	11	-1	965	898
17	1	736	745	21	14	995	1106	26	14	633	549	11	1	623	597
17	4	888	969	21	16	760	560	26	15	633	590	11	3	645	627
17	6	2070	2303	22	-2	3170	3539	26	16	441	458	11	4	421	392
17	8	713	856	22	-1	1594	1859	26	18	439	447	11	5	499	390
17	13	517	500	22	0	846	919	27	-2	207	531	11	7	1065	1067
18	-2	2311	2850	22	2	1432	1572	27	-1	1809	2001	11	9	962	1079
18	-1	638	850	22	3	1449	1465	27	0	291	138	12	-3	1781	1799
18	0	828	1003	22	5	2115	2131	27	4	3972	4029	12	-1	942	916

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	3****		19	4	491	430	23	9	729	630	27	10	572	673
12	1	469	420	19	5	2148	2592	23	13	792	743	27	12	1343	1394
12	4	626	500	19	7	817	825	23	15	492	518	27	14	1737	1589
12	5	398	359	19	9	510	499	24	-3	882	843	27	16	890	955
12	7	546	458	19	13	587	495	24	-2	2483	2527	28	-3	208	66
12	8	447	548	20	-3	5521	5875	24	-1	1310	1419	28	-2	2677	2219
12	10	627	616	20	-1	3003	3167	24	0	528	590	28	-1	826	1013
13	-3	503	536	20	0	463	406	24	1	752	799	28	0	1049	1142
13	-2	1103	1132	20	1	940	1014	24	2	504	414	28	1	3017	3033
13	2	472	640	20	2	682	822	24	3	681	686	28	2	464	529
13	3	538	542	20	4	1561	1842	24	4	2424	2851	28	3	4071	3886
13	4	675	637	20	5	1438	1484	24	5	712	838	28	5	333	303
13	5	1269	1384	20	6	1044	1119	24	6	2474	2596	28	6	1273	1241
13	6	744	698	20	7	713	933	24	7	588	576	28	7	491	531
13	7	585	701	20	8	492	641	24	8	538	431	28	8	1674	1665
14	-3	1781	2002	20	11	950	1050	24	12	666	704	28	10	1198	1242
14	-2	737	716	20	13	1789	1837	24	13	615	520	28	11	1292	1259
14	-1	951	1085	20	15	1277	1316	24	15	585	650	28	13	1658	1628
14	4	520	516	21	-3	1078	1135	25	-3	1617	1648	28	15	467	471
14	6	932	1084	21	-1	1028	746	25	-1	863	1123	28	16	740	726
15	-2	777	913	21	0	2074	2496	25	1	653	939	28	17	426	397
15	0	758	705	21	2	1802	1944	25	3	1788	1917				
15	2	625	689	21	3	1486	1555	25	4	768	800		**H =	4****	
15	3	539	493	21	4	882	1075	25	5	1890	2065	0	-2	7144	6652
15	5	519	564	21	5	2232	2531	25	6	1035	779	0	0	2525	2079
15	7	545	580	21	6	501	409	25	7	1053	911	0	2	4694	4670
16	-3	722	788	21	7	1114	1291	25	8	530	564	0	6	1302	1270
16	2	502	434	21	8	558	736	25	9	508	433	0	8	434	507
16	4	805	840	21	10	854	916	25	10	557	425	0	10	1604	1817
16	6	921	1063	21	12	1244	1321	25	12	825	812	0	12	2446	2345
16	7	691	763	21	15	610	631	25	14	1145	1113	0	14	1906	1771
16	8	452	380	21	16	549	544	26	-3	2392	2582	0	16	1229	1309
16	13	614	779	22	-3	1665	1787	26	-2	1052	1139	0	18	573	832
17	-3	808	716	22	-2	1090	1048	26	-1	860	594	7	-3	346	121
17	-2	551	731	22	-1	830	718	26	0	610	622	8	-4	670	681
17	1	363	460	22	0	724	794	26	1	369	394	8	-3	675	670
17	2	1069	1087	22	1	948	921	26	3	430	580	8	-1	486	378
17	3	838	915	22	2	525	615	26	4	1433	1464	8	0	432	317
17	4	910	959	22	4	1679	1953	26	5	833	694	9	-3	856	931
17	5	1220	1196	22	6	3406	3525	26	6	1336	1424	9	3	375	341
17	7	612	641	22	7	795	628	26	7	1029	1004	10	-4	1755	1831
17	10	538	677	22	8	1642	1723	26	9	790	710	10	-2	571	532
17	12	884	919	22	9	577	410	26	11	1075	1082	10	2	456	359
17	14	468	603	22	11	768	722	26	12	613	632	10	3	858	914
18	-2	522	521	22	13	1119	1074	26	13	816	768	10	5	693	762
18	1	376	375	22	14	676	662	26	15	548	492	10	6	371	423
18	2	1127	1360	22	15	1107	1204	26	17	547	542	11	-4	616	658
18	3	682	791	22	16	638	718	27	-3	1197	1300	11	-3	1203	1316
18	4	2365	2833	22	17	574	613	27	-2	3080	3223	11	-2	664	608
18	6	2216	2667	23	-2	446	389	27	-1	334	331	11	-1	486	532
18	7	517	667	23	-1	2144	2393	27	0	2020	1661	11	0	447	269
18	8	817	850	23	0	652	399	27	2	1113	1029	11	1	843	817
19	-3	489	658	23	3	774	981	27	3	2281	2434	11	2	404	435
19	-2	1572	1722	23	4	948	1029	27	4	2541	2755	11	3	916	1068
19	-1	990	1095	23	5	519	523	27	5	4096	4395	11	4	789	865
19	0	895	986	23	7	512	495	27	6	1528	1456	11	6	404	424
19	3	1366	1539	23	8	700	632	27	7	1901	2057	12	-4	1289	1296
												12	-2	697	760



K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
12	-4	1054	955	18	6	832	954	23	-2	831	887	28	-3	822	602
12	-3	882	916	19	-5	432	356	23	-1	359	346	28	-2	3128	2957
12	2	607	541	19	-4	1258	1179	23	1	506	525	28	-1	1110	1000
12	4	671	724	19	-3	521	497	23	2	461	533	28	0	908	651
12	5	702	741	19	-2	1310	1425	23	3	698	727	28	1	3857	3626
12	6	415	513	19	0	576	653	23	4	483	484	28	2	2360	2230
13	-5	767	746	19	1	984	1192	23	5	683	811	28	3	2327	2522
13	-4	1302	1300	19	2	536	593	23	6	775	807	28	4	1310	1443
13	-3	662	601	19	3	1427	1627	23	7	782	811	28	6	2033	2453
13	-2	738	750	19	7	1069	1372	24	-5	759	678	28	8	1808	2003
13	0	410	381	19	9	727	872	24	-4	567	564	28	9	991	989
13	2	647	697	19	12	702	758	24	-2	584	645	28	11	1165	1204
13	3	782	784	19	14	545	739	24	0	1222	1292	28	14	463	515
13	5	653	743	20	-5	3976	4059	24	1	655	701				
14	-5	1571	1593	20	-4	962	815	24	2	429	510				
14	-4	936	942	20	-3	1815	1802	24	3	600	704				
14	-3	1470	1470	20	-2	820	877	24	4	2707	2803				
14	-2	621	608	20	-1	1583	1666	24	6	637	770				
14	-1	667	689	20	0	493	530	24	9	497	411				
14	2	636	632	20	1	538	585	25	-5	1179	1162				
14	4	703	712	20	2	1117	1501	25	-4	1787	1910				
14	5	482	330	20	4	1866	2108	25	-3	306	158				
14	6	713	870	20	7	550	562	25	-2	1751	1843				
15	-5	617	666	20	8	704	863	25	-1	1195	1256				
15	-4	1323	1350	20	9	827	909	25	0	387	371				
15	0	906	937	20	11	1264	1421	25	2	1128	1198				
15	2	938	1011	20	13	1273	1383	25	3	1326	1412				
15	5	533	530	20	15	625	762	25	5	1492	1549				
15	6	496	536	21	-5	1608	1769	25	7	751	706				
15	7	743	933	21	-4	752	602	25	15	492	302				
15	12	541	529	21	-3	1001	1051	26	-5	1113	1367				
16	-5	1168	1360	21	-2	1065	1173	26	-3	1361	1276				
16	-4	787	850	21	-1	390	509	26	-2	1695	1652				
16	-1	506	526	21	0	1173	1261	26	-1	2437	2442				
16	1	628	778	21	2	549	1069	26	0	1305	1257				
16	2	745	983	21	3	2118	2343	26	1	632	628				
16	3	524	603	21	5	2146	2556	26	3	927	985				
16	4	1213	1475	21	6	954	1092	26	4	1031	1137				
16	6	688	806	21	7	486	513	26	7	536	403				
16	7	575	572	21	10	847	847	26	9	929	1133				
16	13	413	415	22	-5	1785	1770	26	11	914	905				
17	-5	1740	1453	22	-4	611	668	27	-5	1026	958				
17	-4	1133	1220	22	-2	527	521	27	-4	4406	4065				
17	0	1186	1155	22	0	556	555	27	-3	3373	3277				
17	2	911	945	22	1	372	375	27	-1	1689	1765				
17	3	885	1016	22	2	1113	1137	27	0	1825	1721				
17	5	709	767	22	4	2487	2864	27	2	968	864				
17	10	725	891	22	6	1354	1510	27	3	2325	2413				
17	12	718	916	22	7	693	774	27	4	1092	1192				
18	-2	415	493	22	8	608	517	27	5	1790	1989				
18	-1	376	255	22	9	1213	1432	27	6	548	840				
18	0	770	775	22	11	1081	1154	27	8	719	764				
18	1	435	460	22	12	741	640	27	10	1240	1349				
18	2	1073	1379	22	13	1010	1004	27	12	1143	995				
18	4	1800	2164	22	14	695	810	27	14	676	674				
18	5	833	1068	23	-5	730	731	28	-5	658	621				
				23	-4	616	723	28	-4	1000	880				



Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
13	6	635	715	19	12	551	661	24	4	499	361	28	15	649	685
13	7	421	601	20	-6	2102	2058	24	5	532	601	28	16	559	724
13	8	771	1005	20	-5	2406	2380	24	6	738	814	**H = 7****			
14	-6	617	708	20	-3	1529	1462	24	12	1009	1036	0	-6	1726	1749
14	-5	705	770	20	-2	874	784	24	14	642	557	0	-4	1920	1716
14	-4	817	815	20	-1	2123	2186	25	-6	1790	1726	0	-2	1704	1512
14	0	483	550	20	0	783	862	25	-5	1525	1573	0	0	1823	1998
14	1	463	561	20	1	2834	2994	25	-4	805	718	0	2	8176	8340
14	3	838	944	20	3	4065	4623	25	-3	411	549	0	4	4645	4942
14	5	1045	1205	20	5	1855	2300	25	-2	321	265	0	6	960	1194
14	6	499	466	20	7	746	973	25	0	1676	1821	0	10	449	222
14	7	444	413	20	8	822	953	25	1	945	1018	0	12	640	725
15	-6	1032	1066	20	10	731	926	25	3	421	316	0	14	500	624
15	-5	646	641	21	-6	1319	1193	25	4	1253	1235	0	16	593	499
15	-4	656	706	21	-5	1010	892	25	10	570	518	9	-6	497	656
15	2	1098	1288	21	-4	1256	1286	26	-6	617	523	9	-5	472	417
15	4	1079	1176	21	-3	2404	2502	26	-5	668	501	9	-4	531	395
16	-5	1164	1228	21	-2	497	519	26	-4	984	1012	9	-1	461	534
16	-3	579	563	21	-1	1138	1129	26	-3	2275	2210	9	1	828	904
16	3	985	963	21	0	519	439	26	-2	550	651	9	3	438	349
16	4	433	443	21	3	572	469	26	0	769	831	10	-7	596	604
17	-5	1335	1470	21	4	1251	1653	26	1	433	510	10	-3	548	480
17	-2	393	409	21	5	715	806	26	2	1146	1233	10	-2	716	808
17	-1	969	940	21	6	1908	2376	26	3	1528	1430	10	-1	730	821
17	0	563	755	21	11	676	645	26	4	386	419	10	0	1385	1516
17	2	1233	1372	21	12	537	734	26	7	804	1130	10	2	1231	1376
17	4	644	740	22	-6	3203	3151	27	-6	1314	1222	10	4	348	335
17	6	604	667	22	-5	493	601	27	-5	820	767	10	5	414	516
17	8	567	750	22	-4	1861	2012	27	-4	679	594	11	-6	676	759
17	10	479	638	22	-2	1216	1241	27	-3	2965	2890	11	-5	836	760
18	-6	3289	3424	22	0	1085	1126	27	-2	714	650	11	-3	1252	1160
18	-5	938	966	22	1	1205	1353	27	-1	2260	2204	11	-2	440	342
18	-4	1435	1481	22	2	649	720	27	0	401	376	11	-1	992	1042
18	-3	541	379	22	3	2583	2757	27	1	1276	1288	11	1	1173	1278
18	-1	583	543	22	4	1251	1191	27	2	3918	3986	11	3	543	658
18	0	1137	1106	22	5	913	1155	27	3	826	1117	12	-7	1834	1777
18	1	486	533	22	7	625	734	27	4	4030	4486	12	-6	768	617
18	3	866	827	22	10	564	526	27	5	888	903	12	-5	1355	1366
18	4	526	526	22	12	941	988	27	7	829	801	12	-4	725	641
18	7	503	584	22	14	574	731	27	9	867	913	12	-2	490	518
18	12	437	526	23	-6	1555	1570	27	10	517	530	12	2	406	305
19	-6	1299	1355	23	-5	855	876	27	11	709	658	12	3	450	334
19	-5	2501	2567	23	-3	907	970	27	12	507	630	13	-6	889	783
19	-4	1069	1016	23	-2	507	561	27	13	769	902	13	-5	1130	1106
19	-2	1259	1403	23	-1	1191	1065	27	14	449	613	13	-4	594	580
19	-1	1556	1627	23	0	439	464	28	-6	928	882	13	-3	457	416
19	0	1389	1420	23	1	1045	1095	28	-4	355	18	13	-2	458	508
19	1	1714	2037	23	2	918	935	28	-3	1021	1174	13	0	603	579
19	2	1204	1334	23	15	556	731	28	-2	971	1047	13	1	1029	1173
19	3	464	610	24	-6	3060	3231	28	0	1219	1094	13	3	625	661
19	4	1079	1346	24	-5	397	383	28	1	1185	1187	13	7	384	353
19	5	582	588	24	-4	1149	1136	28	2	1165	1483	14	-7	895	718
19	6	805	1056	24	-3	993	990	28	3	708	842	14	-6	611	651
19	7	703	769	24	-2	505	557	28	4	671	753	14	-5	627	526
19	9	1358	1570	24	-1	327	513	28	5	888	1027	14	-4	799	902
19	11	840	1137	24	0	941	946	28	7	1548	1516	14	-1	1047	1100
				24	3	638	699	28	14	1145	1297	14	0	554	595



Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
		**H = 7****		20	11	1214	1538	25	1	1314	1321	0	8	1507	1592
14	1	1006	1006	20	13	528	806	25	2	966	934	0	10	2850	2946
14	2	564	578	21	-7	922	806	25	3	1183	1265	0	12	1886	1977
14	7	380	224	21	-6	372	267	26	-7	2568	2448	8	-7	575	528
14	9	576	680	21	-5	1632	1632	26	-6	810	819	8	-5	695	646
15	-6	1694	1734	21	-4	399	334	26	-5	465	473	8	-2	507	606
15	-4	561	624	21	-3	1221	1307	26	-4	838	941	9	-7	942	900
15	0	478	609	21	-1	874	926	26	-3	1150	956	9	-5	405	443
15	1	450	359	21	0	668	1079	26	-2	553	576	9	-2	514	616
15	2	574	548	21	1	1156	1211	26	-1	2521	2690	9	0	587	699
16	-7	1127	1177	21	3	1703	1783	26	0	370	205	9	1	381	425
16	-5	475	599	21	5	1047	1158	26	1	1873	1969	10	-8	772	754
16	-2	493	438	21	14	784	997	26	2	447	437	10	-6	399	540
16	-1	880	956	22	-7	3135	3174	26	3	715	1121	10	-1	463	470
16	0	461	391	22	-6	564	575	26	5	769	864	10	0	389	316
16	2	639	727	22	-5	1661	1780	26	15	455	526	10	1	435	580
16	4	675	770	22	-4	1542	1585	27	-7	599	710	11	-8	934	718
17	-7	1017	1030	22	-3	533	422	27	-6	4807	4308	11	-2	416	388
17	-6	1405	1540	22	-1	676	807	27	-5	2396	2274	11	0	873	880
17	-5	1426	1413	22	0	1496	1678	27	-4	1559	1491	11	2	374	410
17	-2	616	557	22	1	829	995	27	-3	443	310	11	3	492	463
17	0	661	719	22	2	2876	3073	27	-2	611	537	11	4	509	625
17	1	481	652	22	3	436	555	27	-1	415	495	11	5	443	271
17	3	581	643	22	4	1493	1669	27	0	1315	1466	12	-4	418	306
17	10	779	942	22	5	695	633	27	1	948	966	12	-2	636	780
17	12	424	591	22	6	523	731	27	2	812	780	12	-1	1216	1288
18	-7	1094	1116	22	7	561	586	27	3	1369	1308	12	0	414	676
18	-6	1648	1464	22	8	580	601	27	4	535	771	12	1	1598	1740
18	-4	771	696	22	9	952	1177	27	8	948	973	12	2	454	317
18	-2	579	667	22	11	1282	1332	27	10	1230	1231	12	3	875	919
18	0	2392	2518	23	-7	2159	2106	27	12	877	962	12	6	405	288
18	2	2438	2681	23	-5	1083	1080	28	-6	3672	3469	13	-6	523	548
18	3	664	697	23	-4	331	343	28	-5	649	591	13	-4	589	649
18	4	675	806	23	-3	444	437	28	-4	362	134	13	-2	977	932
19	-7	421	299	23	-2	746	719	28	-3	832	758	13	0	1082	1146
19	-6	933	911	23	0	394	257	28	-2	1406	1256	13	2	726	809
19	-5	626	619	23	2	1005	1039	28	-1	839	284	13	4	526	643
19	-2	481	479	23	3	1647	1941	28	0	1386	1312	13	5	551	543
19	-1	722	881	23	4	789	989	28	1	1468	1515	13	6	442	470
19	0	1156	1251	23	5	1640	1702	28	2	485	228	13	8	383	424
19	1	1933	2026	24	-7	1150	1123	28	3	415	351	14	-8	797	719
19	3	553	570	24	-6	752	632	28	4	1978	2076	14	-7	820	726
19	5	1180	1350	24	-5	509	485	28	5	413	277	14	-6	919	880
19	7	888	1121	24	-4	1768	1725	28	6	2318	2667	14	-5	465	333
19	9	706	769	24	-3	766	642	28	8	1241	1302	14	-4	588	728
19	10	503	761	24	-1	744	681	28	10	587	730	14	-3	462	478
19	12	481	578	24	1	958	1125	28	13	563	745	14	1	641	707
20	-7	3642	3618	24	2	2686	2726	28	14	481	508	14	2	633	650
20	-6	912	953	24	3	1013	1122	28	15	529	549	14	3	872	902
20	-5	2012	2092	24	4	1584	1913			**H = 8****		14	5	496	641
20	-4	1112	1159	24	5	541	566	0	-6	7710	7249	14	9	423	590
20	0	1016	941	25	-7	2718	2436	0	-4	2512	2526	15	-8	857	786
20	2	1654	1669	25	-6	1759	1665	0	-2	1662	1805	15	-6	1233	1323
20	5	1016	1197	25	-5	1366	1322	0	0	494	321	15	0	1606	1755
20	6	749	867	25	-2	473	354	0	2	598	665	15	1	444	145
20	7	631	807	25	-1	852	732	0	4	2043	2151	15	2	1405	1584
20	9	585	788	25	0	1821	2008	0	6	1749	1764	15	4	489	629

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	8****		21	-2	491	533	26	-1	2106	2015	11	-3	1038	1105
16	-8	882	929	21	0	1086	1019	26	0	1114	1181	11	-1	933	1123
16	-7	1469	1451	21	2	449	533	26	1	1666	1641	11	1	702	923
16	-5	577	410	21	4	1859	2196	26	3	402	82	11	2	459	577
16	-1	576	804	21	6	689	1040	26	7	919	1157	11	3	445	590
16	1	774	849	21	8	667	864	26	9	838	973	12	-9	1115	1078
16	2	656	684	21	9	567	649	27	-8	385	295	12	-8	433	438
16	3	437	393	22	-8	3081	2769	27	-7	1048	911	12	-7	1151	1003
16	5	665	826	22	-7	1276	1303	27	-6	680	464	12	-5	590	499
17	-7	724	703	22	-6	1559	1440	27	-4	742	801	12	-1	405	484
17	-6	610	430	22	-5	957	1074	27	-3	625	628	13	-9	777	707
17	-3	914	842	22	-4	491	475	27	-2	2234	2392	13	-8	800	797
17	-2	601	765	22	-3	514	480	27	-1	2360	2433	13	-7	642	642
17	-1	1385	1573	22	-1	1416	1355	27	0	3523	3300	13	-5	756	778
17	0	1145	1297	22	1	2114	2141	27	2	3011	3195	13	-3	442	430
17	2	792	1026	22	2	815	985	27	3	806	940	13	-2	732	737
17	5	495	451	22	3	920	1083	27	4	850	998	13	-1	1303	1400
17	8	577	699	22	7	730	1053	27	5	786	968	13	1	733	899
18	-8	2786	2798	22	9	548	546	27	6	445	398	14	-9	1301	1326
18	-7	1275	1141	22	10	977	1172	27	7	505	546	14	-8	533	498
18	-6	1566	1549	22	12	630	898	27	8	502	230	14	-7	676	673
18	-5	574	567	23	-8	1183	1051	27	9	922	992	14	-6	738	612
18	-2	1055	1029	23	-7	639	554	27	11	803	900	14	-5	434	430
18	2	883	977	23	-6	694	688	28	-7	1845	1868	14	-2	721	814
18	6	609	652	23	-5	370	146	28	-6	876	644	14	0	633	848
18	8	684	879	23	-2	351	246	28	-5	1002	998	15	-8	947	1013
18	10	717	874	23	0	1131	1130	28	-3	856	1112	15	-6	1235	1170
19	-8	745	859	23	2	803	910	28	-2	642	911	15	8	485	616
19	-7	1514	1306	23	3	817	769	28	-1	1209	1122	16	-9	1415	1338
19	-5	500	557	23	13	755	776	28	0	316	283	16	-7	810	882
19	-3	1558	1562	24	-8	2455	2199	28	2	949	1052	16	-6	486	377
19	-2	1431	1548	24	-7	441	541	28	3	1858	1956	16	-5	658	772
19	-1	2408	2640	24	-6	1236	1174	28	5	1759	1971	16	-3	582	300
19	0	783	893	24	-2	1033	996	28	7	1131	1325	16	0	631	443
19	1	536	632	24	0	666	665	28	9	941	775	16	1	1011	1092
19	2	933	1076	24	1	453	639	28	12	1198	1598	16	2	502	335
19	4	800	873	24	2	628	645	28	13	560	674	16	7	691	774
19	9	787	938	24	3	446	479	28	14	979	1317	16	9	509	631
19	10	560	806	24	4	700	713					17	-8	778	747
20	-8	2477	2395	24	6	883	904		**H =	9****		17	-7	1742	1758
20	-7	1666	1616	24	10	997	1052	0	-8	1291	1296	17	-5	775	858
20	-6	1385	1434	24	-7	1942	1746	0	-6	3780	3756	17	-4	613	639
20	-5	2343	2360	25	-6	353	131	0	-4	2641	2773	17	-4	613	639
20	-4	408	383	25	-6	673	561	0	2	2638	2629	17	-2	853	983
20	-3	2083	2216	25	-5	973	331	0	0	5532	5284	17	-1	697	823
20	-2	420	415	25	-4	845	761	0	2	4771	5209	17	1	566	638
20	-1	4226	4394	25	-3	737	669	0	4	1853	2212	17	4	457	512
20	1	4146	4502	25	-2	1611	1518	0	8	478	525	17	6	497	594
20	3	1469	1809	25	0	717	879	0	14	593	593	17	8	523	519
20	6	617	811	25	1	871	1009	9	-1	784	813	18	-9	1696	1460
20	8	874	938	25	2	1008	1133	10	-9	493	472	18	-8	502	456
20	10	510	675	25	3	748	952	10	-7	415	550	18	-7	677	519
21	-8	1997	1978	25	6	630	630	10	-3	403	384	18	-6	450	636
21	-7	1365	1374	25	9	833	735	10	-2	795	894	18	-4	1258	1406
21	-6	1721	1770	26	-8	993	873	10	0	1031	1190	18	-2	2634	2726
21	-5	558	409	26	-7	942	883	11	-8	744	670	18	-1	561	706
21	-4	443	282	26	-5	1790	1920	11	-7	801	807	18	0	2752	3008
				26	-3			11	-5	1148	1179	18	1	870	1023

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 9****				23	-6	436	481	27	5	863	935	13	-2	680	753
18	2	832	869	23	-5	1268	904	27	6	806	928	13	0	855	875
18	3	475	645	23	-3	952	1008	27	7	549	678	13	2	550	595
19	-8	657	586	23	-1	1063	1031	27	8	1801	2044	13	3	417	388
19	-7	428	413	23	0	624	601	27	10	1216	1430	14	-10	1034	896
19	-6	422	467	23	2	545	540	27	13	467	344	14	-9	574	597
19	-1	1973	2082	23	3	1160	1324	28	-9	600	493	14	-8	935	840
19	0	567	458	23	4	497	693	28	-8	1941	2026	14	-6	619	621
19	1	808	953	23	5	696	889	28	-7	398	279	14	-3	665	652
19	3	502	601	23	7	830	1042	28	-6	1917	1744	14	-2	537	474
19	5	1075	1252	23	17	721	589	28	-5	1190	1233	14	-1	1146	1130
19	7	985	1147	24	-9	1352	1188	28	-3	975	1102	14	0	690	786
19	10	439	731	24	-8	703	556	28	-2	2495	1990	14	1	690	738
20	-9	3178	2898	24	-7	462	416	28	-1	399	385	14	5	401	368
20	-7	1446	1556	24	-6	1431	1391	28	0	1266	1148	15	-10	659	507
20	-3	563	566	24	-4	1854	2021	28	2	795	679	15	-8	1254	1134
20	-2	1021	1082	24	-3	368	438	28	3	835	869	15	-6	607	592
20	-1	479	458	24	-2	1225	1170	28	4	1157	1405	15	-5	517	555
20	0	680	693	24	-1	439	360	28	6	1507	1794	15	-2	872	899
20	3	958	989	24	0	1695	1816	28	7	720	792	15	0	1373	1564
20	4	654	646	24	1	835	853	28	8	941	1052	15	2	955	1063
20	5	1383	1584	24	2	1402	1491	28	13	625	771	15	3	449	289
20	7	1117	1363	24	4	689	738	28	17	1305	963	16	-10	479	353
20	9	1313	1827	24	17	1113	973	**H = 10****				16	-9	1284	1235
21	-9	856	930	24	18	522	365	0	-8	5057	4686	16	-8	594	609
21	-8	552	508	25	-9	2233	2058	0	-6	3241	3136	16	-7	1024	1049
21	-7	401	237	25	-8	1335	1296	0	-5	496	0	16	-3	766	790
21	-6	1307	1305	25	-7	1897	1906	0	-4	548	548	16	-1	598	848
21	-4	1030	1205	25	-6	1383	1425	0	-2	715	687	16	5	683	763
21	-3	1123	1211	25	-4	395	380	0	0	571	685	17	-9	576	475
21	-2	511	670	25	-3	847	844	0	2	1552	1448	17	-7	763	820
21	-1	2023	2076	25	-2	495	448	0	4	1775	2155	17	-3	504	536
21	0	1014	1127	25	-1	1513	1587	0	6	1888	1922	17	-2	1316	1437
21	1	1643	1818	25	2	900	884	0	8	2893	2867	17	-1	611	636
21	3	1380	1521	25	3	514	453	0	10	2336	2599	17	0	518	691
21	5	669	723	25	7	642	646	9	-7	617	596	18	-10	2574	2369
21	8	856	736	25	8	714	902	9	-4	591	529	18	-9	925	940
21	12	720	989	25	18	373	359	10	-10	630	612	18	-8	2153	2055
22	-9	2777	2538	26	-9	1043	698	11	-10	783	721	18	-7	648	679
22	-7	1885	1809	26	-6	394	320	11	-8	526	504	18	-6	1029	1023
22	-6	1584	1647	26	-5	1018	858	11	-3	554	683	18	-3	706	815
22	-5	900	932	26	-4	492	477	11	-2	816	991	18	-1	548	392
22	-4	1517	1616	26	-3	2266	2240	11	0	508	674	18	0	727	822
22	-3	561	711	26	-1	593	516	11	1	534	520	18	6	1116	1447
22	-2	1800	1687	26	0	488	604	11	3	622	704	18	8	1103	1373
22	0	2954	3170	26	3	465	467	12	-10	443	428	19	-10	1540	1478
22	1	626	482	27	-9	764	662	12	-7	461	472	19	-9	843	876
22	2	1872	2057	27	-8	5501	5011	12	-6	558	604	19	-6	420	201
22	3	858	916	27	-7	1685	1534	12	-5	533	502	19	-5	883	897
22	4	965	996	27	-6	2647	2646	12	-3	805	775	19	-3	1489	1564
22	5	641	758	27	-5	2056	2022	12	-1	1163	1307	19	-2	741	792
22	7	773	774	27	-4	1124	1095	12	1	1040	1073	19	0	793	976
22	8	608	301	27	-2	487	468	12	3	383	259	19	1	451	451
22	9	1463	1782	27	-1	2730	2871	13	-9	831	901	19	2	995	1210
23	-9	1712	1518	27	0	1614	1673	13	-8	613	609	19	3	672	720
23	-8	1113	1014	27	1	368	486	13	-6	754	685	19	4	525	551
23	-7	1568	1487	27	4	400	438	13	-4	818	781	19	5	726	882

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 10****				23	11	533	755	27	3	486	499	15	-2	568	491
19	7	707	922	23	16	758	666	27	5	610	757	15	0	691	818
20	-10	1298	1323	23	17	760	624	27	7	1055	1225	15	1	404	268
20	-9	841	899	24	-10	1737	1495	27	8	662	780	15	2	584	557
20	-8	1381	1506	24	-9	1400	1275	27	9	743	953	15	6	594	746
20	-7	1857	1947	24	-8	1884	1740	27	19	402	287	16	-11	661	669
20	-5	1945	2032	24	-7	459	300	28	-10	357	297	16	-9	880	858
20	-3	3233	3356	24	-6	989	879	28	-9	1635	1599	16	-7	540	675
20	-1	2505	2960	24	-5	510	428	28	-8	920	1068	16	-4	585	508
20	0	1011	1123	24	-2	1096	993	28	-7	2262	2168	16	-3	482	509
20	1	2073	2405	24	1	526	438	28	-6	1294	1313	16	-2	956	914
20	6	845	981	24	2	1392	1501	28	-4	1106	1245	16	-1	1030	1101
20	8	457	601	24	6	611	648	28	-3	1624	1520	16	1	695	621
20	9	537	697	24	7	576	719	28	-2	570	318	16	5	629	712
20	16	371	130	24	8	1178	1207	28	0	1320	1554	16	7	551	642
21	-10	1588	1576	24	10	689	703	28	3	951	1109	17	-11	756	642
21	-9	2028	1838	24	16	445	306	28	4	722	699	17	-10	1131	957
21	-8	1733	1726	24	19	1233	920	28	5	1638	1774	17	-9	754	688
21	-7	483	458	25	-10	1215	1050	28	6	861	677	17	-6	649	676
21	-6	961	914	25	-9	1756	1628	28	7	604	778	17	-4	1018	979
21	-5	773	876	25	-8	653	618	28	10	928	1266	17	-1	520	587
21	-4	850	703	25	-7	1035	1094	28	12	1135	1499	17	3	503	612
21	-3	1110	1229	25	-6	438	237	28	19	408	323	17	4	699	946
21	-2	790	718	25	-2	1149	1178	**H = 11****				17	6	467	801
21	2	589	729	25	-1	1416	1485	0	-10	1313	1176	17	7	474	436
21	4	824	971	25	0	793	1035	0	-8	2568	2442	17	16	992	880
21	6	714	923	25	1	1510	1641	0	-6	1940	2023	18	-9	710	813
21	9	580	845	25	4	649	664	0	-4	3792	3908	18	-6	1278	1319
21	17	480	470	25	6	720	841	0	-2	4830	4725	18	-4	1103	1217
22	-10	2292	2134	25	7	657	809	0	0	3957	4131	18	-2	1905	2182
22	-9	1197	1102	25	9	602	705	0	2	1233	1326	18	-1	898	1056
22	-8	1745	1664	25	16	540	336	0	8	582	570	18	0	1403	1588
22	-7	1254	1287	25	18	561	476	0	12	454	475	18	1	554	680
22	-6	1491	1498	25	19	384	340	10	-4	679	769	18	6	457	439
22	-5	581	606	26	-7	738	730	10	-2	911	1007	18	16	478	366
22	-4	951	910	26	-5	665	607	11	-10	691	789	19	-9	491	334
22	-3	1741	1618	26	-3	828	813	11	-9	475	447	19	-4	561	632
22	-2	683	690	26	-2	392	322	11	-8	698	715	19	-3	983	960
22	-1	1731	1869	26	0	713	770	11	-7	890	911	19	-2	509	590
22	1	433	507	26	2	520	606	11	-5	735	766	19	-1	784	794
22	2	541	531	26	5	495	299	12	-11	1173	1060	19	3	902	917
22	4	681	718	26	10	480	251	12	-10	1018	960	19	5	779	855
22	5	832	868	26	16	1281	1046	12	-6	510	547	19	8	477	724
22	8	1231	1492	26	17	412	314	12	-3	411	452	19	16	551	453
22	10	766	1019	26	18	626	493	12	-2	433	346	20	-11	3002	2683
22	17	690	567	27	-10	387	331	13	-8	451	481	20	-10	475	287
23	-10	518	490	27	-9	1201	1168	13	-4	571	636	20	-9	2394	2227
23	-8	799	753	27	-8	370	304	13	-3	698	741	20	-8	465	381
23	-7	378	313	27	-7	920	899	13	-1	816	924	20	-7	966	1053
23	-6	795	739	27	-6	1108	1098	13	0	437	520	20	-6	464	356
23	-2	1011	1000	27	-4	3080	2938	13	4	378	369	20	-4	1270	1307
23	-1	524	661	27	-3	1287	1300	14	-11	1319	1101	20	-2	1125	1341
23	0	800	859	27	-2	4495	4645	14	-10	453	488	20	-1	710	834
23	1	420	548	27	-1	473	443	14	-2	676	765	20	1	985	1016
23	5	554	560	27	0	2331	2331	14	0	656	768	20	2	793	871
23	7	697	774	27	1	580	592	15	-10	861	948	20	3	1255	1323
23	10	537	643	27	2	731	543	15	-6	718	545	20	5	1418	1760

Table 45. Continued

**H = 11****								**H = 12****							
K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
20	7	1252	1780	24	-10	1039	872	27	6	1517	1784	14	-1	474	462
20	9	794	1242	24	-9	596	429	27	8	1277	1687	14	0	514	653
21	-11	1565	1435	24	-6	545	484	27	15	381	207	15	-12	762	804
21	-10	447	533	24	-5	1546	1407	27	16	470	264	15	-10	639	585
21	-9	1044	986	24	-4	1568	1534	27	17	704	547	15	-7	515	558
21	-8	1310	1276	24	-3	1248	1185	27	18	767	590	15	-5	643	565
21	-7	549	524	24	-2	1484	1521	28	-10	1441	1454	15	-4	598	528
21	-6	571	532	24	0	1296	1316	28	-9	725	656	15	-2	1296	1379
21	-5	394	196	24	2	571	564	28	-8	2200	2144	15	0	731	878
21	-4	811	851	24	15	1374	1171	28	-6	632	765	15	15	623	542
21	-3	1926	1927	24	16	731	630	28	-5	1623	1681	16	-11	912	895
21	-2	942	997	24	17	579	502	28	-3	416	292	16	-9	1224	1013
21	-1	1677	1850	25	-11	1711	1655	28	-1	528	471	16	-7	513	453
21	0	681	612	25	-10	883	910	28	2	530	551	16	-5	535	538
21	1	930	1028	25	-9	2327	2141	28	3	732	737	16	-3	639	748
21	3	476	481	25	-8	1018	974	28	4	732	705	16	-1	520	479
21	4	693	781	25	-7	966	834	28	5	752	775	16	4	401	329
21	6	818	750	25	-5	765	674	28	11	569	959	16	16	426	291
21	8	519	390	25	-4	500	475	28	15	1967	1449	17	-9	605	607
21	10	837	1101	25	-3	1274	1376	28	17	864	663	17	-4	643	768
21	15	986	742	25	-1	619	728					17	-3	1044	1040
21	16	1053	879	25	6	640	680	0	-10	2408	2205	17	-2	495	580
21	18	493	377	25	7	508	617	0	-8	1757	1675	17	-1	577	681
22	-11	1374	1198	25	8	503	558	0	-4	341	101	18	-12	2189	1834
22	-10	478	359	25	15	395	317	0	-2	758	689	18	-11	619	601
22	-9	1296	1241	25	18	548	364	0	2	2266	2308	18	-10	1346	1398
22	-8	625	621	25	19	893	649	0	4	2216	2341	18	-9	793	758
22	-6	1128	1062	26	-10	1197	1018	0	6	1841	2224	18	-8	899	973
22	-5	537	561	26	-9	1690	1653	0	8	1717	2124	18	-5	1122	1158
22	-4	1877	1710	26	-8	689	636	10	-6	778	724	18	-3	1272	1243
22	-3	385	238	26	-7	471	467	11	-12	462	287	18	-3	1272	1243
22	-2	1810	1825	26	-3	445	523	11	-11	511	511	18	2	673	788
22	0	1905	2073	26	0	439	436	11	-10	724	708	18	4	867	1086
22	1	724	875	26	1	578	928	11	-8	438	398	18	6	914	1135
22	2	850	812	26	3	625	703	11	-5	531	515	19	-12	815	665
22	3	924	998	26	5	751	842	11	-4	610	678	19	-11	1264	1139
22	5	663	706	26	6	461	678	11	-2	411	399	19	-10	1537	1391
22	6	698	758	26	11	539	694	12	-2	411	399	19	-9	821	693
22	7	1053	1222	26	17	390	408	12	-9	701	638	19	-8	503	504
22	9	496	776	26	18	722	501	12	-7	591	570	19	-7	859	805
22	17	668	568	26	-5	890	898	12	-5	890	898	19	-5	1175	1222
22	18	653	448	26	-3	1023	1225	12	-3	1023	1225	19	-4	605	607
22	19	1089	930	26	-1	814	855	12	-1	814	855	19	-2	506	475
23	-10	1606	1531	27	-11	2240	2129	13	-11	862	813	19	1	575	655
23	-9	1249	1095	27	-10	3594	3443	13	-10	664	557	19	3	939	1197
23	-8	1373	1252	27	-9	1336	1320	13	-9	682	737	19	5	781	984
23	-7	891	885	27	-8	2258	2293	13	-8	733	713	19	15	1738	1345
23	-3	450	529	27	-7	692	627	13	-2	607	641	19	17	972	676
23	0	866	813	27	-6	433	253	13	0	655	869	19	18	570	388
23	3	456	538	27	-5	510	549	13	2	466	550	20	-12	1044	991
23	15	875	721	27	-3	808	983	14	-12	930	901	20	-11	697	657
23	16	578	526	27	-2	1936	2074	14	-11	1169	1111	20	-10	566	454
23	17	967	771	27	-1	1580	1824	14	-10	915	763	20	-9	1038	1086
23	18	697	511	27	1	451	431	14	-9	1000	960	20	-8	630	600
23	19	612	506	27	2	1239	1135	14	-8	445	383	20	-7	1262	1284
24	-11	1252	1082	27	3	883	872	14	-5	506	572	20	-6	502	622
				27	4	1013	1072	14	-3	878	859	20	-5	1396	1488
				27	5	658	780	14	-2	512	534	20	-4	423	233

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 12***				24	-12	1598	1401	27	-2	3395	3673	13	0	532	506
20	-3	2139	2273	24	-11	1535	1463	27	0	1385	1437	14	-13	616	438
20	-2	648	621	24	-10	1647	1538	27	1	814	836	14	-12	641	442
20	-1	2081	2277	24	-9	997	934	27	2	518	497	14	-11	460	310
20	0	572	698	24	-8	848	816	27	4	577	628	14	-8	453	204
20	1	754	938	24	0	903	1013	27	6	933	1056	14	-7	549	688
20	2	555	452	24	2	1129	1075	27	7	560	616	14	-4	504	568
20	5	449	475	24	5	463	445	27	14	623	474	14	-3	493	560
20	7	521	578	24	6	1215	1330	27	16	602	396	14	-2	543	514
20	18	618	473	24	7	572	753	27	17	736	646	14	-1	709	771
21	-12	836	737	24	8	855	1090	27	18	1183	928	14	0	577	723
21	-11	1034	719	24	15	539	355	27	19	658	505	14	14	561	524
21	-10	1983	1801	24	19	1585	1226	27	20	1267	950	15	-12	788	641
21	-9	1278	1179	24	20	424	312	28	-12	1231	1018	15	-2	642	654
21	-8	629	459	25	-12	737	718	28	-11	468	381	15	0	641	766
21	-3	499	654	25	-11	1308	1186	28	-10	1751	1735	15	3	497	518
21	5	613	775	25	-10	686	576	28	-9	642	715	15	13	531	342
21	7	918	1168	25	-9	1259	1132	28	-8	994	1032	15	14	620	516
21	15	700	550	25	-8	589	580	28	-7	801	840	16	-11	995	1057
21	16	477	441	25	-7	697	588	28	-6	1432	1316	16	-6	475	483
21	17	553	312	25	-3	1516	1522	28	-5	653	632	16	-4	815	708
21	18	487	355	25	-2	1245	1291	28	-4	1408	1354	16	-3	1185	1179
22	-12	2468	2091	25	-1	1378	1622	28	-3	551	546	16	-1	625	722
22	-10	1412	1255	25	1	705	841	28	-2	1291	1351	16	5	437	547
22	-9	480	425	25	2	541	624	28	-1	469	408	16	14	1026	920
22	-8	794	788	25	5	481	622	28	0	979	1111	16	16	514	316
22	-6	1489	1491	25	7	601	558	28	2	761	767	17	-13	793	747
22	-5	1237	1279	25	16	666	571	28	3	673	800	17	-12	764	748
22	-4	844	976	25	17	1183	972	28	4	1273	1366	17	-11	508	451
22	-3	2056	2308	25	18	702	567	28	5	840	920	17	-9	598	608
22	-1	812	766	25	19	564	493	28	7	621	545	17	-7	1005	878
22	0	728	911	26	-12	404	445	28	8	614	721	17	-6	866	905
22	2	1222	1231	26	-11	840	806	28	10	828	1122	17	-3	582	594
22	3	756	756	26	-10	451	430	28	17	869	729	17	0	487	543
22	4	710	711	26	-9	1386	1153	28	19	858	653	17	4	680	891
22	6	886	1106	26	-7	1058	982	**H = 13***				17	14	1482	1192
22	8	1018	1338	26	-6	432	351	0	-12	1130	996	17	16	561	446
22	14	736	615	26	-5	1145	949	0	-10	1083	1016	17	17	626	451
22	19	814	656	26	-4	449	453	0	-8	1396	1460	18	-9	628	458
23	-12	474	385	26	-3	711	765	0	-6	1082	1144	18	-8	755	784
23	-10	988	816	26	-2	615	581	0	-4	4448	4843	18	-6	1218	1200
23	-9	471	469	26	-1	386	225	0	-2	4057	4267	18	-4	1782	1857
23	-8	680	533	26	0	827	896	0	0	1413	1518	18	-3	620	706
23	-7	416	391	26	1	473	548	0	2	463	335	18	-2	1264	1343
23	-6	389	336	26	2	911	1019	0	6	451	526	18	4	451	483
23	-5	712	754	26	14	2815	2221	11	-9	545	605	18	6	505	679
23	-4	445	541	26	15	507	240	11	-7	542	591	18	13	608	394
23	-2	784	856	26	16	1438	1234	12	-13	899	736	18	17	743	573
23	-1	921	891	26	19	525	291	12	-12	826	829	19	-11	559	464
23	3	654	566	26	20	612	546	12	-11	596	550	19	-5	514	503
23	5	621	591	27	-11	578	445	12	-10	760	731	19	-3	469	306
23	8	493	681	27	-9	550	626	12	-5	389	502	19	1	753	820
23	9	523	657	27	-8	525	536	13	-8	571	551	19	3	681	741
23	14	725	701	27	-6	1967	1926	13	-6	582	602	19	4	676	834
23	15	689	689	27	-5	997	1056	13	-5	490	533	19	13	648	618
23	16	711	607	27	-4	3639	3897	13	-3	573	573	19	14	965	795
23	18	573	444	27	-3	1316	1579	13	-2	407	386	20	-13	2284	1825

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	13****		23	-9	528	348	26	-2	430	404	0	2	768	1023
20	-12	473	382	23	-8	714	643	26	1	520	707	0	4	1588	1960
20	-11	766	573	23	-7	1283	1206	26	5	530	486	0	6	1635	2028
20	-10	541	548	23	-5	621	566	26	6	650	679	12	-11	437	454
20	-9	516	518	23	-4	504	544	26	8	513	771	12	-9	423	446
20	-8	736	662	23	-2	1087	1130	26	14	657	564	12	-7	732	831
20	-6	800	874	23	0	623	539	26	15	448	544	12	-5	928	1004
20	-4	1831	1892	23	1	480	459	26	17	953	651	12	-3	442	538
20	-2	771	975	23	4	468	432	26	18	815	633	12	12	764	606
20	-1	825	937	23	5	440	255	26	19	889	690	13	-12	503	456
20	0	536	522	23	9	465	241	26	20	884	577	13	-10	766	734
20	1	986	1087	23	14	981	881	27	-13	1156	1021	13	-8	676	634
20	2	531	622	23	16	766	563	27	-12	1990	1803	13	-6	478	481
20	3	854	1121	23	19	590	414	27	-11	1326	1255	13	-1	427	526
20	5	1043	1416	23	20	586	527	27	-10	1386	1303	13	13	842	632
20	7	848	1027	24	-13	1023	840	27	-8	1003	1017	14	-14	882	735
20	17	435	472	24	-12	566	506	27	-7	387	353	14	-13	1000	800
20	18	543	447	24	-11	875	815	27	-6	394	394	14	-12	962	806
20	19	436	457	24	-9	1013	919	27	-3	1237	1215	14	-11	793	723
21	-13	1399	1195	24	-8	733	771	27	-2	805	904	14	-10	569	512
21	-12	465	348	24	-7	1026	1061	27	-1	584	699	14	-9	780	640
21	-11	2354	2085	24	-5	1011	1123	27	0	904	851	14	-5	639	609
21	-10	1341	1267	24	-4	1665	1609	27	2	701	754	14	-4	628	579
21	-9	1400	1305	24	-3	789	948	27	4	1141	1323	14	-3	511	606
21	-6	1407	1489	24	-2	1480	1527	27	6	1334	1382	14	-2	422	471
21	-5	588	660	24	0	667	816	27	8	535	675	14	12	671	587
21	-3	1014	1070	24	13	1663	1339	27	13	526	683	14	13	610	449
21	-2	1171	1250	24	14	519	489	27	16	600	460	14	15	579	487
21	-1	554	530	24	15	1063	881	27	18	725	496	15	-14	1116	906
21	13	1203	1107	24	16	631	493	27	20	415	272	15	-12	795	742
21	14	1553	1276	24	17	698	488	28	-12	1456	1386	15	-7	612	586
21	15	627	514	24	19	406	272	28	-11	495	380	15	-6	724	771
21	16	1120	938	25	-13	1686	1520	28	-10	1806	1688	15	-4	1153	1186
21	17	572	556	25	-12	537	540	28	-9	1101	1062	15	-2	456	588
21	19	793	606	25	-11	1969	1926	28	-8	1063	930	15	13	606	567
22	-13	1555	1358	25	-10	450	461	28	-7	940	980	16	-14	953	681
22	-11	905	951	25	-9	1180	1192	28	-6	679	556	16	-13	1156	1055
22	-8	710	745	25	-7	558	529	28	-5	831	719	16	-11	794	752
22	-7	776	801	25	-6	949	976	28	-1	401	405	16	-8	595	603
22	-6	1623	1670	25	-5	963	1111	28	0	644	702	16	-7	450	517
22	-5	1390	1481	25	-4	762	676	28	1	436	606	16	-5	837	895
22	-4	1753	1882	25	-3	1460	1498	28	3	686	699	16	12	1066	858
22	-2	1403	1463	25	4	610	556	28	4	623	459	16	13	753	649
22	-1	464	274	25	5	609	810	28	7	543	524	16	16	647	525
22	0	581	745	25	13	1005	858	28	9	500	643	17	-14	445	182
22	1	617	691	25	15	1366	1126	28	13	3068	2456	17	-7	553	719
22	2	533	479	25	16	527	415	28	15	1875	1571	17	-6	521	568
22	3	619	749	25	17	447	465	28	17	886	679	17	-4	633	614
22	5	631	820	25	19	711	628	28	19	1086	870	17	-3	518	558
22	13	491	363	26	-13	611	471	28	21	1159	908	17	2	625	661
22	17	986	817	26	-11	479	377		**H =	14****		17	4	419	413
22	18	778	599	26	-10	1028	963	0	-12	1638	1229	17	14	448	229
22	20	768	627	26	-9	1159	1008	0	-10	1214	1133	17	17	451	385
23	-13	1149	1117	26	-8	359	400	0	-8	388	250	17	18	587	544
23	-12	873	705	26	-7	812	875	0	-6	2478	2528	18	-14	986	1010
23	-11	1500	1290	26	-5	1440	1511	0	-4	442	165	18	-13	670	603
23	-10	1176	1030	26	-3	693	687	0	0	793	813	18	-12	725	698



Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 14****															
18	-11	570	636	22	-9	598	519	25	20	406	164	0	2	470	460
18	-8	794	664	22	-6	941	972	26	-13	671	625	12	11	762	689
18	-5	636	692	22	-5	1832	1861	26	-11	503	474	13	-8	462	472
18	-4	630	676	22	-4	936	819	26	-9	913	986	13	-7	792	853
18	0	498	694	22	-3	1336	1443	26	-8	473	501	13	-5	598	631
18	2	519	666	22	-2	528	681	26	-6	871	924	14	-14	416	303
18	4	687	936	22	0	578	671	26	-5	1211	961	14	-12	613	479
18	13	760	677	22	2	502	625	26	-2	779	905	14	-9	490	523
18	14	571	451	22	3	502	612	26	0	501	581	14	-8	745	746
18	17	438	393	22	4	758	904	26	1	438	549	14	-6	619	612
18	18	488	391	22	6	801	1027	26	2	505	569	14	-3	559	589
19	-13	816	637	22	12	874	686	26	7	405	29	14	-1	459	456
19	-12	884	895	22	13	544	492	26	12	3112	2695	14	12	708	479
19	-11	558	597	22	14	801	769	26	14	1806	1567	14	15	632	521
19	-10	1155	1083	22	15	438	228	26	15	585	383	15	-15	466	306
19	-9	553	426	22	17	456	369	26	20	667	557	15	-8	729	760
19	-8	919	866	23	-11	502	391	27	-10	488	330	15	-2	471	663
19	-7	1559	1513	23	-7	1513	1574	27	-9	579	630	15	11	494	411
19	-6	603	664	23	-6	648	648	27	-8	734	859	15	15	831	759
19	-3	471	447	23	-5	506	505	27	-7	1186	1240	16	-15	921	813
19	3	656	808	23	-4	1043	1087	27	-6	2569	2676	16	-13	1009	944
19	13	1135	944	23	-3	1105	1134	27	-5	1045	1374	16	-11	812	743
19	14	428	400	23	-2	441	330	27	-4	3241	3400	16	-9	611	560
19	15	728	577	23	-1	621	696	27	-3	757	905	16	-5	1165	1249
19	16	450	347	23	6	561	532	27	-2	1287	1458	16	-4	663	670
19	17	628	580	23	12	987	814	27	4	596	653	16	-3	975	1010
19	18	1050	810	23	13	1153	991	27	5	508	550	16	11	491	419
19	19	731	424	23	14	1087	861	27	6	420	601	16	12	940	803
20	-14	1130	1005	23	18	569	459	27	14	560	421	16	13	835	688
20	-13	949	718	23	19	440	236	27	15	582	600	16	14	602	510
20	-12	899	748	24	-14	938	813	27	16	518	508	17	-15	408	386
20	-11	1088	876	24	-11	494	481	27	17	853	707	17	-13	531	586
20	-10	552	464	24	-9	424	360	27	18	1063	950	17	-11	433	285
20	-9	1227	1063	24	-8	1035	982	27	19	429	333	17	-9	463	507
20	-8	444	319	24	-6	1075	985	28	-13	879	880	17	-8	568	654
20	-7	2034	1989	24	-5	648	750	28	-12	712	692	17	-6	462	492
20	-5	2263	2174	24	-2	1050	1121	28	-11	447	385	17	-2	446	471
20	-3	1247	1215	24	4	1160	1216	28	-8	900	1052	17	3	411	421
20	2	428	552	24	6	861	1108	28	-6	956	1086	17	11	672	654
20	16	917	715	24	7	448	465	28	-4	973	993	17	12	1590	1349
20	18	972	739	24	14	443	235	28	-3	906	997	17	15	542	340
21	-14	1201	976	24	15	573	354	28	-2	1482	1812	17	17	765	598
21	-12	1559	1218	24	17	1261	1142	28	-1	516	539	18	-15	1082	911
21	-11	475	410	24	19	1308	1043	28	3	696	534	18	-11	416	391
21	-9	758	672	24	20	598	518	28	6	564	691	18	-8	1478	1529
21	-6	633	406	25	-13	1000	915	28	7	500	478	18	-7	488	538
21	1	567	709	25	-9	443	544	28	13	1101	947	18	-6	1943	2012
21	2	551	683	25	-7	565	671	28	19	918	540	18	-4	854	1054
21	3	958	1112	25	-6	502	523	28	21	851	680	18	11	775	571
21	5	585	800	25	-5	1221	1202	**H = 15****				18	14	456	438
21	13	932	784	25	-4	954	894	0	-14	1346	1219	18	15	633	546
21	19	847	609	25	-3	1559	1700	0	-12	2109	1837	18	16	637	503
21	20	466	358	25	-1	670	652	0	-10	890	777	18	17	540	383
22	-14	1625	1359	25	8	468	528	0	-8	1121	1169	19	-8	597	468
22	-13	838	693	25	15	1533	1322	0	-6	2616	2559	19	-7	712	725
22	-12	442	218	25	16	627	647	0	-4	2733	2665	19	-1	518	630
				25	17	1277	965	0	-2	1440	1586	19	1	667	813



K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	15****		22	-4	1006	1014	25	3	570	791	28	15	779	662
19	3	418	495	22	-3	491	392	25	4	486	685	28	19	1000	838
19	11	940	857	22	-2	653	747	25	5	639	907	28	21	667	449
19	12	496	469	22	0	491	322	25	11	492	539	**H = 16****			
19	13	634	388	22	3	744	776	25	13	1091	901	0	-14	1119	801
19	15	606	416	22	11	492	508	25	15	501	401	0	-12	638	641
19	16	515	353	22	13	1087	949	25	16	639	536	0	-8	1155	1145
19	17	442	314	22	15	1670	1309	25	17	725	560	0	-4	954	1060
19	19	485	338	22	16	485	365	25	19	419	254	0	-2	977	1327
20	-15	978	853	22	17	2102	1642	26	-14	465	252	0	0	898	1037
20	-11	671	524	22	18	818	746	26	-10	424	459	0	2	1944	2073
20	-10	776	798	22	19	409	432	26	-9	1247	1230	0	4	1350	1738
20	-9	515	434	22	20	410	356	26	-7	806	909	0	6	445	548
20	-6	824	869	23	-15	1415	1203	26	-3	528	628	10	10	956	924
20	-4	635	733	23	-14	528	541	26	3	465	311	11	10	593	314
20	-3	748	799	23	-13	1868	1519	26	12	709	708	11	11	1115	1071
20	-1	854	1056	23	-12	783	673	26	15	667	542	12	10	663	621
20	0	476	565	23	-11	1037	921	26	16	850	774	12	12	691	681
20	1	568	952	23	-5	455	400	26	17	1455	1148	12	14	821	725
20	3	873	1054	23	-4	1163	1215	26	18	1323	1007	13	11	643	550
20	5	621	858	23	-3	653	664	26	19	934	750	13	13	479	491
20	11	865	624	23	-2	1170	1310	26	20	1383	1091	13	14	650	572
20	12	793	701	23	1	642	705	26	21	480	389	13	15	642	659
20	13	597	468	23	2	599	579	27	-15	673	653	14	-12	552	503
20	14	461	264	23	5	428	456	27	-14	1345	1113	14	-11	394	293
20	15	930	747	23	11	607	551	27	-13	1217	1063	14	-7	608	598
20	16	954	815	23	12	926	779	27	-12	431	486	14	-6	479	432
20	17	1025	879	23	18	795	728	27	-11	392	293	14	-5	620	630
20	18	580	542	23	19	512	494	27	-9	448	282	14	10	769	659
20	19	669	569	23	20	762	633	27	-8	469	296	14	16	454	420
21	-13	1156	1108	24	-14	1006	885	27	-5	450	416	15	-14	1103	952
21	-12	887	715	24	-13	612	485	27	-2	634	799	15	-12	480	392
21	-11	1059	982	24	-12	788	652	27	0	736	1026	15	-11	518	461
21	-9	824	872	24	-11	703	771	27	4	1133	1247	15	-9	779	680
21	-8	1563	1602	24	-9	550	607	27	7	427	443	15	-8	837	741
21	-7	836	830	24	-8	964	998	27	14	648	504	15	-6	595	644
21	-5	896	900	24	-7	738	778	27	15	593	482	15	10	483	335
21	-4	1006	1079	24	-6	1008	947	27	16	1085	758	15	11	774	696
21	-3	548	543	24	-5	1645	1724	27	17	443	314	15	15	947	778
21	-2	511	615	24	-4	878	909	27	18	1127	890	16	-15	628	471
21	2	594	576	24	-3	731	691	27	21	494	358	16	-14	483	335
21	12	2323	2039	24	-2	1003	1133	28	-15	427	308	16	-13	733	666
21	13	488	392	24	11	1958	1770	28	-14	1009	838	16	-9	617	586
21	14	1186	1090	24	12	497	446	28	-13	493	410	16	-7	679	666
21	16	537	457	24	15	441	351	28	-12	973	878	16	10	1242	1116
21	17	568	514	24	16	806	616	28	-9	474	529	16	11	489	380
21	19	597	501	24	17	992	747	28	-8	943	841	16	12	458	42
22	-15	1363	1098	25	-15	873	812	28	-7	502	475	16	14	441	380
22	-14	990	845	25	-13	1483	1333	28	-6	834	588	16	15	551	422
22	-13	745	674	25	-11	705	636	28	-5	582	660	17	-16	425	380
22	-12	1212	1105	25	-8	1393	1428	28	0	1226	1524	17	-15	529	488
22	-10	1218	1142	25	-7	937	902	28	2	1032	1010	17	-9	574	658
22	-9	637	588	25	-6	773	794	28	4	480	500	17	-8	762	822
22	-8	1946	1886	25	-5	1191	1248	28	5	521	646	17	0	442	565
22	-7	671	735	25	-3	593	587	28	7	458	716	17	10	533	561
22	-6	2012	1959	25	1	458	339	28	11	2368	2001	17	14	829	768
22	-5	575	447	25	2	604	692	28	13	2486	2112	17	15	628	480

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	16****		21	3	504	638	25	-15	1174	1098	28	-1	1011	1015
17	16	1416	1199	21	10	517	464	25	-13	902	945	28	1	670	723
17	17	709	525	21	11	614	445	25	-9	515	466	28	6	442	698
17	18	811	651	21	17	582	453	25	-8	836	829	28	13	486	387
18	-16	999	863	21	18	807	654	25	-7	1256	1292	28	17	803	639
18	-15	546	501	21	19	830	729	25	-5	1170	1379	28	19	2089	1460
18	-14	796	758	21	20	745	536	25	-3	642	580	28	21	1014	762
18	-13	553	520	22	-16	1043	848	25	-2	630	687			**H =	17****
18	-12	693	706	22	-15	1011	896	25	0	711	696	0	-16	1402	1155
18	-10	575	460	22	-9	606	527	25	1	492	541	0	-14	1593	1364
18	-6	419	448	22	-8	587	551	25	10	763	698	0	-12	1358	1135
18	-5	454	507	22	-7	667	603	25	13	694	699	0	-10	1924	1768
18	-3	560	501	22	-6	508	661	25	15	1017	896	0	-8	2014	1947
18	0	541	768	22	-2	482	589	26	-16	428	23	0	-6	1207	1201
18	2	848	1085	22	-1	625	625	26	-11	475	470	0	-4	699	567
18	10	1007	945	22	0	724	735	26	-9	704	522	0	0	512	677
18	11	930	877	22	1	484	573	26	-8	622	550	10	9	457	474
18	12	944	829	22	2	696	745	26	-7	472	491	10	11	914	865
18	14	675	468	22	4	509	633	26	-6	776	807	11	9	630	692
18	15	928	813	22	10	611	535	26	-5	460	578	11	11	772	721
18	17	520	513	22	11	708	733	26	-4	804	885	11	12	607	598
18	18	490	437	22	12	836	763	26	-3	449	308	12	9	1154	1063
19	-13	548	617	22	13	532	557	26	1	891	1121	12	11	451	351
19	-12	571	496	22	14	506	323	26	10	2735	2487	13	9	538	501
19	-10	551	490	22	15	1195	917	26	11	674	699	13	10	804	763
19	-9	901	880	22	17	856	737	26	12	1453	1378	13	14	465	149
19	-8	654	728	23	-13	943	763	26	15	773	636	14	11	475	206
19	-6	490	521	23	-11	541	519	26	17	496	363	15	-10	413	541
19	11	1998	1677	23	-9	951	1050	26	18	453	423	15	-8	425	586
19	13	538	524	23	-8	823	836	26	20	492	446	15	-6	573	550
19	15	516	461	23	-6	948	884	27	-16	430	348	15	9	500	493
19	16	730	676	23	-5	998	1161	27	-12	921	855	15	11	533	355
19	17	789	693	23	-4	936	1010	27	-10	1462	1431	15	13	513	526
19	18	878	772	23	-3	558	475	27	-9	769	786	15	15	1471	1288
19	19	1017	749	23	4	514	647	27	-8	2296	2229	15	17	874	719
20	-16	909	836	23	10	962	825	27	-7	931	965	16	-13	819	893
20	-15	683	582	23	11	1014	906	27	-6	1426	1510	16	-7	742	728
20	-14	803	864	23	12	475	463	27	-5	939	846	16	-5	796	875
20	-13	846	801	23	15	474	394	27	-4	793	891	16	10	559	505
20	-11	832	810	23	16	831	686	27	1	614	712	16	11	709	486
20	-9	2114	2011	23	18	760	561	27	2	470	566	16	13	618	518
20	-7	2115	2112	24	-16	825	608	27	13	713	594	16	14	957	827
20	-6	465	355	24	-10	613	638	27	14	1221	895	16	16	450	372
20	-5	938	1045	24	-9	624	419	27	15	1465	1262	16	17	704	516
20	-1	417	312	24	-4	631	713	27	16	1637	1434	17	-15	545	394
20	0	448	593	24	2	971	986	27	17	1432	1143	17	-13	433	373
20	2	608	708	24	4	537	699	27	20	596	517	17	-12	469	405
20	11	923	780	24	11	633	540	28	-15	960	858	17	-10	737	690
20	14	1421	1091	24	12	422	321	28	-14	731	695	17	-1	428	400
20	16	1477	1244	24	13	515	367	28	-13	762	752	17	10	2154	2023
20	18	991	821	24	14	608	515	28	-10	947	955	17	12	548	405
21	-14	682	649	24	15	741	666	28	-9	819	724	17	17	592	460
21	-12	552	542	24	17	1387	1109	28	-8	662	619	18	-17	656	588
21	-8	843	620	24	18	432	291	28	-5	850	958	18	-16	440	556
21	-2	504	664	24	19	976	780	28	-4	1084	1304	18	-15	890	752
21	0	856	936	24	20	781	607	28	-3	428	564	18	-10	991	1092
21	1	505	649	24	21	531	468	28	-2	950	1146	18	-8	1230	1244

Table 45, Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 17****				22	-17	808	724	25	-15	712	599	28	-10	533	411
18	-7	550	676	22	-15	873	723	25	-14	838	719	28	-2	1285	1305
18	-6	887	1053	22	-14	878	770	25	-13	664	640	28	0	615	747
18	-5	411	545	22	-12	1394	1244	25	-11	648	555	28	9	3136	2756
18	-2	582	636	22	-11	610	566	25	-9	1124	1025	28	11	1615	1645
18	10	1185	989	22	-10	1571	1464	25	-8	452	601	28	13	984	860
18	12	666	621	22	-8	1165	1100	25	-7	667	597	28	15	1311	973
18	14	574	422	22	-6	781	714	25	-6	562	640	28	17	950	765
19	-12	491	378	22	-5	542	566	25	-5	520	619	28	19	747	632
19	-9	453	413	22	-1	657	546	25	1	416	521	28	21	497	219
19	-4	552	491	22	1	679	794	25	3	616	799	**H = 18****			
19	-1	636	742	22	10	605	468	25	13	1101	716	0	-16	1422	1081
19	10	572	520	22	11	470	428	25	15	1300	964	0	-14	892	738
19	11	884	760	22	12	870	751	25	17	441	289	0	-6	873	902
19	12	704	517	22	13	1644	1461	25	20	605	423	0	-4	1280	1421
19	14	554	393	22	14	580	576	25	21	1069	904	0	-2	994	1013
19	15	930	838	22	15	2449	1997	26	-15	602	468	0	0	1250	1547
19	16	488	298	22	16	551	468	26	-13	525	315	0	2	1031	1400
19	17	823	517	22	17	1296	1127	26	-11	748	668	0	4	581	723
19	19	770	603	22	18	776	632	26	-9	525	586	9	8	414	435
20	-17	957	807	23	-16	837	726	26	-3	492	402	9	10	565	653
20	-15	750	652	23	-15	718	684	26	0	490	721	10	8	1020	1005
20	-11	597	588	23	-14	787	753	26	1	468	312	10	12	424	405
20	-10	397	352	23	-13	803	873	26	12	389	314	11	8	635	586
20	-8	591	574	23	-9	576	521	26	14	1616	1500	11	9	1062	1031
20	-5	651	606	23	-6	688	584	26	15	1302	1116	11	11	451	268
20	-3	555	660	23	-4	732	777	26	16	1491	1227	11	13	503	381
20	-2	436	489	23	-2	424	504	26	17	1265	1073	12	8	734	649
20	-1	933	1077	23	-1	761	924	26	18	1417	1071	12	9	586	479
20	1	759	1000	23	2	443	445	26	20	1233	1028	12	10	1183	1094
20	9	1819	1567	23	9	1604	1387	27	-17	1258	1053	12	12	934	890
20	10	459	437	23	10	754	682	27	-16	1417	1183	12	13	539	631
20	11	794	712	23	11	1366	1185	27	-15	1058	935	12	14	718	686
20	13	764	701	23	13	621	588	27	-14	1129	1028	13	9	749	674
20	14	1773	1509	23	15	611	450	27	-8	679	638	13	11	594	420
20	15	1296	1019	23	16	1327	1080	27	-5	571	532	13	13	684	583
20	16	1144	1006	23	18	899	761	27	-4	832	944	13	14	1013	950
20	17	826	752	23	19	603	444	27	-3	533	653	13	15	746	642
20	19	438	433	23	21	604	491	27	-2	1081	1198	14	8	873	798
20	20	670	451	24	-17	528	440	27	-1	876	1027	14	9	481	380
21	-17	566	491	24	-16	833	748	27	0	1282	1565	14	10	605	615
21	-16	462	301	24	-13	714	603	27	2	886	1245	14	14	562	425
21	-14	567	593	24	-11	622	589	27	9	502	419	14	16	885	704
21	-11	509	359	24	-10	1318	1329	27	10	375	338	15	9	1169	1051
21	-10	660	735	24	-9	723	716	27	11	438	450	15	11	621	487
21	-9	780	822	24	-8	734	775	27	12	1076	876	15	13	814	817
21	-7	877	954	24	-7	673	731	27	13	658	488	15	15	578	460
21	-5	563	546	24	-5	443	452	27	14	1096	927	16	-9	474	611
21	10	2725	2316	24	0	613	769	27	15	1823	1564	16	-8	424	396
21	12	1015	896	24	9	1737	1522	27	16	1041	772	16	-7	420	561
21	13	796	566	24	10	794	665	27	17	749	616	16	8	710	642
21	14	459	475	24	11	742	668	27	18	612	573	16	13	783	772
21	15	1014	892	24	13	597	554	27	21	897	779	16	18	421	308
21	16	622	600	24	14	1276	1035	28	-15	747	723	17	-10	453	505
21	17	633	485	24	15	1119	965	28	-14	535	588	17	-9	552	557
21	18	625	588	24	16	841	723	28	-12	621	618	17	9	823	821
21	19	500	300	25	-17	453	343	28	-11	509	275	17	12	1009	915

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 18****				21	10	608	411	24	10	1157	884	28	-10	680	660
17	13	1257	1112	21	11	563	425	24	11	779	707	28	-6	532	611
17	14	1362	1090	21	12	651	718	24	13	1718	1446	28	-2	524	350
17	15	1226	1046	21	14	900	957	24	15	958	746	28	-1	536	656
17	16	1026	771	21	15	1327	1158	24	17	1092	816	28	9	2621	2383
17	17	587	593	21	16	1388	1120	24	19	801	766	28	13	1957	1728
17	18	929	769	21	17	660	662	25	-18	963	828	28	15	1294	866
18	-15	494	429	21	18	818	696	25	-17	1713	1429	28	17	1449	1056
18	-14	657	643	21	20	680	560	25	-16	703	650	28	19	1329	1041
18	-4	407	392	22	-18	1058	826	25	-15	1502	1269	**H = 19****			
18	8	858	741	22	-17	566	451	25	-9	903	994	0	-14	505	462
18	9	1023	961	22	-16	821	637	25	-7	958	1162	0	-12	1183	1173
18	12	608	602	22	-15	448	360	25	-5	652	910	0	-10	1745	1764
18	13	2273	1922	22	-11	645	660	25	-2	436	607	0	-8	1822	1809
18	14	963	745	22	-9	776	784	25	1	463	521	0	-6	670	658
18	15	1525	1340	22	-6	682	719	25	8	989	845	8	7	860	838
18	16	713	647	22	-4	1045	1166	25	10	1390	1286	9	8	540	548
18	18	632	497	22	-2	918	1040	25	11	986	928	9	9	596	626
19	-15	472	350	22	0	485	657	25	13	605	547	10	7	968	920
19	9	3963	3532	22	8	1208	1051	25	16	562	417	10	8	469	401
19	11	1400	1245	22	9	1400	1283	26	-15	1100	1083	10	9	1040	1027
19	12	1181	864	22	11	1086	1123	26	-13	744	734	10	11	981	1004
19	13	808	623	22	13	638	574	26	-11	480	363	10	12	748	727
19	14	801	761	22	16	468	145	26	-9	465	328	11	7	646	688
19	15	820	707	22	19	551	468	26	-7	484	356	11	9	1050	1033
19	16	587	529	23	-17	767	581	26	-6	845	825	11	10	528	433
19	17	711	542	23	-15	918	875	26	-4	703	862	11	13	612	563
19	18	691	556	23	-14	760	666	26	-3	497	621	12	7	1125	1190
19	19	467	415	23	-10	665	610	26	-1	582	702	12	8	692	660
20	-17	460	433	23	-8	435	495	26	8	5358	4869	12	9	1056	998
20	-16	900	758	23	-7	416	448	26	9	1357	1279	13	8	873	716
20	-15	610	547	23	-6	631	687	26	10	2223	2012	13	9	609	420
20	-14	552	573	23	-5	479	491	26	19	582	414	13	11	500	319
20	-13	597	508	23	9	961	827	27	-18	464	531	14	8	729	681
20	-12	422	274	23	10	498	489	27	-16	512	362	14	9	529	484
20	-11	911	894	23	11	596	599	27	-12	1593	1482	14	10	575	485
20	-9	1270	1326	23	12	1403	1162	27	-10	1893	1900	14	11	1083	941
20	-7	873	933	23	14	1455	1255	27	-9	575	605	14	12	455	432
20	-5	417	434	24	-18	714	596	27	-8	1243	1305	14	13	648	444
20	-4	427	335	24	-17	541	371	27	-7	784	806	14	14	512	496
20	8	427	199	24	-16	683	499	27	-6	625	648	14	16	470	484
20	9	909	879	24	-13	477	417	27	8	912	845	15	7	549	645
20	12	950	808	24	-12	467	466	27	9	578	503	15	9	509	613
20	14	1617	1186	24	-11	530	538	27	11	551	530	15	12	490	459
20	16	1489	1210	24	-9	437	392	27	12	2066	1796	15	13	1144	1078
20	17	434	364	24	-8	506	457	27	13	815	698	15	15	554	496
20	18	623	609	24	-6	501	523	27	14	2103	1839	15	16	466	337
20	19	797	593	24	5	564	591	27	15	1264	1028	15	17	484	415
21	-14	905	785	24	4	729	791	27	16	706	517	16	7	526	543
21	-11	573	605	24	-3	437	527	27	17	960	798	16	8	806	873
21	-9	578	659	24	-2	830	904	27	20	704	492	16	13	512	380
21	-7	510	613	24	-1	551	675	28	-18	531	510	16	14	1079	984
21	-6	538	496	24	0	744	923	28	-16	1211	1036	16	16	540	363
21	-5	481	498	24	1	463	558	28	-15	537	531	17	7	529	497
21	-2	727	905	24	2	518	478	28	-14	620	631	17	8	3057	2852
21	8	1785	1496	24	8	1120	905	28	-13	578	545	17	10	1338	1278
21	9	1259	1184	24	9	542	507	28	-12	619	495	17	11	486	364

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 19****				22	-12	783	946	25	13	1824	1461	0	-2	718	937
17	12	734	610	22	-11	431	384	25	20	430	179	0	0	1138	1335
18	-12	791	789	22	-10	852	889	25	21	962	794	8	6	433	465
18	-10	747	794	22	-8	475	550	26	-19	465	264	9	8	509	399
18	-9	400	441	22	-4	532	622	26	-18	422	266	10	6	1064	1127
18	-8	775	801	22	-2	473	608	26	-17	1168	909	10	9	380	145
18	7	1608	1528	22	7	578	490	26	-15	586	415	10	12	386	268
18	8	1302	1209	22	10	1026	876	26	-11	631	699	11	7	983	945
18	9	847	776	22	12	1176	1057	26	-3	535	532	11	11	465	511
18	11	1023	885	22	13	704	557	26	-2	428	383	11	13	648	651
18	12	455	456	22	14	707	660	26	0	475	618	12	6	789	695
18	18	464	252	22	15	2166	1762	26	7	1131	1055	12	8	844	837
19	-14	459	321	22	16	693	633	26	8	399	310	12	10	837	836
19	-6	501	606	22	17	525	529	26	11	1091	881	12	11	574	636
19	7	511	285	22	18	641	546	26	12	2573	2345	12	12	727	762
19	8	1254	1331	23	-18	796	650	26	13	1495	1292	12	13	433	321
19	9	465	347	23	-17	515	596	26	14	1733	1381	12	15	874	775
19	10	663	593	23	-16	1064	874	26	15	1496	1242	13	7	821	729
19	13	693	509	23	-15	820	722	26	16	1626	1322	13	10	477	419
19	15	293	917	23	-14	459	430	26	18	1361	1171	13	12	624	626
19	17	597	1284	23	-13	443	377	27	-19	528	412	13	13	926	818
19	19	773	581	23	-1	390	415	27	-18	1291	926	13	14	520	559
20	-15	392	257	23	8	1967	1799	27	-17	708	677	13	15	602	571
20	-12	491	446	23	9	1248	1121	27	-16	1288	1010	13	16	696	499
20	-10	781	913	23	11	1402	1327	27	-15	401	391	14	6	984	990
20	-9	535	443	23	12	469	443	27	-14	418	459	14	7	654	634
20	-7	534	738	23	13	1043	857	27	-6	383	395	14	9	781	800
20	-5	809	870	23	14	485	555	27	-4	628	722	14	10	799	786
20	-3	1007	1091	23	15	653	635	27	-3	687	842	14	12	506	358
20	7	1655	1515	23	20	551	329	27	-2	773	969	14	14	502	345
20	8	475		23	21	427	370	27	0	862	1110	14	16	605	494
20	9	1091		24	-18	375	333	27	9	983	955	15	6	468	462
20	10	1043		24	-17	830	685	27	10	1558	1459	15	7	833	856
20	11	607		24	-15	660	648	27	12	595	628	15	13	849	863
20	12	1586		24	-13	735	724	27	13	910	864	15	15	481	505
20	13	1293		24	-12	575	606	27	14	930	771	16	6	908	964
20	14	1275		24	-11	493	657	27	15	1047	759	16	7	1153	1029
20	15	1239		24	-10	948	1000	27	16	1835	1569	16	8	584	387
20	16	532		24	-8	403	372	27	19	620	603	16	10	826	742
20	20	941		24	7	2729	2336	27	20	962	737	16	11	641	598
21	-17	713		24	8	639	739	27	21	547	536	17	7	1527	1566
21	-16	832		24	9	861	778	28	-16	622	499	17	10	682	706
21	-15	412		24	11	1056	1003	28	-15	658	689	17	11	774	755
21	-14	501		24	12	486	480	28	-14	1062	855	17	12	966	782
21	7	2075		24	13	412	336	28	-12	657	528	17	13	1116	956
21	8	3212		24	14	452	334	28	7	7532	6978	17	14	1516	1261
21	9	1643		24	15	1236	1023	28	9	3270	2948	17	15	570	524
21	10	1546		24	21	745	632	28	11	1843	1430	17	16	1408	1183
21	11	1111		25	-17	548	511	28	13	1747	1519	17	18	575	521
21	12	747		25	-15	593	511	28	15	1685	1394	18	6	593	408
21	13	1598		25	-11	1050	1091	28	17	1163	995	18	7	1948	1838
21	14	550		25	-10	407	248	28	21	855	653	18	8	502	341
21	15	909		25	-9	817	859	**H = 20****				18	9	994	896
21	17	692		25	-7	426	523	0	-16	697	458	18	10	488	487
21	18	509		25	7	405	251	0	-10	641	670	18	11	1793	1728
22	-17	667		25	9	1952	1820	0	-6	620	670	18	12	1231	1086
22	-14	662		25	11	1146	791	0	-4	603	588	18	13	1837	1572

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 20****				23	-12	491	398	26	-6	441	537	10	6	370	100
18	14	1466	1361	23	-10	605	595	26	-4	395	496	10	7	1222	1156
18	15	857	701	23	-9	639	711	26	6	7316	6708	10	9	962	923
18	16	498	463	23	-7	502	597	26	7	759	798	10	10	568	690
18	19	537	559	23	6	399	438	26	8	3280	2954	10	12	579	643
19	7	3455	3426	23	7	851	742	26	10	1104	863	11	8	440	263
19	8	531	458	23	8	1653	1543	26	11	923	860	11	10	683	530
19	9	2246	2049	23	9	879	772	26	12	617	627	11	11	601	529
19	10	747	657	23	10	506	314	26	17	744	634	11	12	737	729
19	11	1768	1665	23	11	553	362	26	19	549	429	11	13	605	660
19	12	1412	1200	23	12	1574	1365	26	20	815	797	11	14	545	613
19	13	1334	1187	23	13	1341	1125	26	21	528	555	12	5	1018	1091
19	14	1071	824	23	14	618	471	27	-15	495	350	12	7	566	600
19	15	567	363	23	16	1115	971	27	-14	384	430	12	8	503	505
19	16	483	375	24	-14	487	418	27	-12	1464	1476	12	14	482	606
20	-13	739	690	24	-13	441	490	27	-11	516	482	12	15	424	300
20	-11	1040	1053	24	-12	620	637	27	-10	1505	1455	13	7	515	352
20	-9	615	647	24	-10	422	418	27	-9	453	594	13	9	665	538
20	-8	395	338	24	-9	476	479	27	-8	638	830	13	10	461	288
20	-7	404	373	24	-7	439	461	27	-6	424	430	13	11	746	587
20	7	830	718	24	-6	423	478	27	7	336	200	14	6	1520	1438
20	10	1078	945	24	-4	521	560	27	8	1888	1530	14	9	790	737
20	11	771	684	24	6	1920	1898	27	9	1426	1407	14	10	560	291
20	12	1140	950	24	7	377	250	27	11	745	671	14	11	1079	1051
20	13	511	456	24	8	619	503	27	12	1477	1287	14	12	564	456
20	14	1658	1468	24	10	1002	828	27	13	682	572	14	14	1038	960
20	16	525	506	24	11	1548	1331	27	14	1175	856	15	5	469	618
20	17	486	512	24	12	888	928	27	15	1048	978	15	6	1379	1251
20	19	701	663	24	13	1362	1135	27	16	554	457	15	8	819	656
20	20	880	766	24	15	1191	941	27	17	539	446	15	10	542	511
21	-5	378	266	24	17	833	713	27	19	586	408	15	11	841	876
21	6	428	196	24	20	1064	849	27	20	503	349	15	13	1207	1055
21	7	2318	2153	24	21	479	232	28	-18	738	567	15	14	500	413
21	8	404	196	25	-17	1215	1116	28	-16	1107	914	15	15	588	608
21	10	544	497	25	-15	890	859	28	-15	451	434	16	5	662	746
21	12	1074	851	25	-12	367	298	28	-14	366	78	16	6	1006	894
21	13	713	610	25	-9	773	854	28	-12	877	801	16	8	845	868
21	14	1794	1493	25	-7	617	679	28	-8	495	551	16	9	899	813
21	15	1001	847	25	-4	444	491	28	-3	549	522	16	10	502	424
21	16	2039	1818	25	-2	469	528	28	7	4227	3913	16	11	777	761
21	17	628	531	25	6	366	205	28	9	2070	1816	16	12	988	848
21	18	693	647	25	7	1394	1315	28	11	3531	2927	16	14	911	810
21	19	457	313	25	8	1084	1081	28	13	2732	2162	17	5	1079	1066
21	20	480	463	25	9	1142	1022	28	15	2193	1719	17	6	2416	2485
22	-12	411	381	25	10	714	650	28	17	1656	1330	17	8	863	869
22	-11	1187	1114	25	11	1142	837	28	21	495	459	17	9	449	514
22	-9	655	768	25	13	661	526	**H = 21****				17	10	499	462
22	-6	615	748	25	18	630	673	0	-12	1362	1246	17	11	685	667
22	-4	572	727	25	19	545	376	0	-10	1552	1461	17	13	522	397
22	6	1236	1261	25	21	750	616	0	-8	795	792	17	17	641	544
22	7	818	755	26	-18	400	210	7	5	620	559	17	18	480	404
22	8	723	632	26	-17	642	578	7	6	391	331	18	5	2357	2504
22	9	1463	1457	26	-16	620	556	8	5	1009	918	18	7	946	825
22	10	419	288	26	-15	920	852	9	5	457	431	18	9	1235	1113
22	12	727	605	26	-14	651	570	9	6	1125	1087	18	11	545	546
22	19	851	845	26	-11	694	560	9	7	465	343	18	15	566	385
23	-15	487	386	26	-9	402	371	10	5	1262	1279	18	19	901	795



Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	21****		23	10	722	414	27	8	2485	2295	14	14	578	521
19	5	2071	1984	23	11	615	568	27	9	806	675	15	4	573	358
19	6	2082	2194	23	13	958	975	27	10	1809	1590	15	5	447	297
19	7	780	622	23	14	557	451	27	11	994	874	15	7	634	725
19	8	563	592	23	15	1066	997	27	12	2161	2087	15	11	670	594
19	9	682	632	23	16	725	702	27	13	1039	832	15	15	489	359
19	10	754	592	23	19	431	465	27	14	1367	1260	16	4	1621	1703
19	11	1058	856	23	20	523	478	27	16	631	394	16	5	1905	1937
19	13	1991	1579	24	-15	681	661	27	17	827	673	16	7	517	435
19	15	2229	1936	24	-13	703	683	27	18	744	706	16	8	900	910
19	17	1006	897	24	-12	821	763	27	19	477	459	16	9	645	632
19	18	436	400	24	-11	429	459	27	20	1481	1182	16	10	621	452
19	19	470	444	24	5	2132	2207	28	-16	508	480	17	4	512	296
20	5	1668	1478	24	6	1162	908	28	-9	493	639	17	5	771	745
20	6	882	900	24	7	377	328	28	-4	514	481	17	8	568	504
20	7	477	417	24	8	537	345	28	5	9095	8563	17	9	645	649
20	8	797	812	24	11	768	553	28	7	6243	5464	17	10	1702	1662
20	10	848	933	24	12	608	605	28	9	2443	2320	17	11	809	674
20	11	1279	1212	24	13	1297	1158	28	11	803	765	17	12	2116	2049
20	12	1153	1048	24	14	565	632	28	13	2194	1925	17	13	600	417
20	13	1743	1467	24	15	507	448	28	15	2327	2098	17	14	1378	1267
20	14	629	365	24	19	454	457	28	17	643	572	18	4	1561	1603
20	15	621	400	24	21	556	448	28	19	642	522	18	5	1933	1804
20	18	553	646	25	-14	664	678	28	21	549	419	18	6	1391	1427
20	20	692	627	25	-13	836	873					18	7	1044	855
21	5	1656	1615	25	-11	1046	1127	0	-12	362	281	18	8	931	742
21	6	3610	3310	25	-9	699	832	0	-8	427	475	18	9	717	704
21	7	2091	2101	25	5	1237	1087	7	5	373	427	18	10	788	819
21	8	1292	1229	25	6	1107	988	8	4	489	572	18	11	1280	1235
21	9	515	409	25	7	2700	2436	8	5	552	503	18	12	1072	1115
21	11	1733	1560	25	8	404	265	8	9	750	773	18	13	773	727
21	13	2223	1892	25	9	1178	992	9	6	482	464	18	14	729	630
21	15	1547	1202	25	10	668	566	10	4	808	1075	19	4	630	545
21	16	844	694	25	11	1003	943	10	8	526	447	19	5	2930	2834
21	20	495	401	25	12	394	274	10	9	521	520	19	7	1815	1771
22	-12	996	1000	25	13	1188	1009	11	5	1353	1435	19	9	1506	1454
22	-10	397	415	25	14	770	687	11	7	717	633	19	10	1537	1328
22	5	877	847	25	16	624	480	11	11	551	522	19	11	1418	1328
22	6	404	407	26	-10	361	277	12	4	924	991	19	12	1456	1240
22	7	2362	2363	26	-9	688	620	12	5	594	677	19	13	1355	1252
22	8	996	902	26	-7	396	463	12	6	618	669	19	14	703	615
22	9	556	505	26	5	1588	1542	12	11	733	676	19	15	1175	1105
22	10	1084	879	26	6	1961	1558	12	12	661	686	19	19	483	373
22	12	1407	1167	26	7	714	611	12	13	693	538	20	4	684	413
22	13	1164	1133	26	8	408	386	12	15	661	651	20	5	1331	1440
22	14	935	797	26	10	2293	2056	13	5	1495	1597	20	6	1245	1157
22	18	435	388	26	11	2008	1759	13	6	443	507	20	8	1525	1388
22	19	933	724	26	12	2784	2374	13	7	575	624	20	9	1043	866
23	-11	408	344	26	13	1843	1608	13	8	544	489	20	10	1972	2056
23	-10	526	469	26	14	2603	2252	13	10	893	813	20	11	1013	946
23	-9	388	278	26	15	1330	1176	13	11	806	764	20	12	1514	1423
23	-8	435	535	26	16	1506	1298	13	12	855	833	20	13	509	454
23	5	394	305	27	-16	538	408	13	13	520	590	20	18	978	790
23	6	2481	2303	27	-6	377	456	14	4	1307	1317	20	19	691	681
23	7	521	421	27	-4	666	802	14	7	507	467	21	4	1359	1327
23	8	584	460	27	6	416	444	14	10	632	688	21	5	1958	1730
23	9	825	732	27	7	1632	1473	14	12	469	403	21	6	418	269

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 22****				26	5	1823	1603	11	8	803	723	19	11	2671	2430
21	7	1320	1215	26	6	3546	3016	11	9	737	771	19	13	2297	2107
21	9	785	696	26	7	328	108	11	10	768	763	19	15	980	899
21	10	999	824	26	8	1093	1001	11	11	534	646	19	16	663	583
21	12	2279	2076	26	9	1594	1484	11	13	693	814	19	18	776	592
21	13	946	1000	26	10	542	421	12	3	1431	1457	20	3	2866	2932
21	14	2488	2162	26	11	1612	1333	12	8	468	500	20	5	2452	2453
21	15	597	701	26	13	1267	953	12	10	636	504	20	6	1600	1428
21	16	1026	983	26	14	1050	958	12	12	435	421	20	7	531	639
21	19	503	438	26	17	961	808	12	14	527	632	20	8	607	626
22	4	692	649	26	18	487	480	13	3	863	914	20	9	942	980
22	5	585	447	26	19	693	603	13	4	551	637	20	10	1945	1716
22	6	692	646	26	20	757	500	13	6	533	509	20	11	917	893
22	7	822	965	26	21	467	481	13	8	466	262	20	13	1001	924
22	10	1359	1059	27	-12	1008	938	13	11	929	832	20	14	961	803
22	11	427	341	27	-10	830	732	13	13	870	739	20	16	948	967
22	12	704	650	27	5	1136	1113	13	15	432	453	20	17	517	596
22	15	637	618	27	6	1425	1333	14	12	607	668	20	18	972	933
22	17	931	985	27	7	1979	1897	15	3	695	753	21	3	909	1114
22	18	552	506	27	8	516	462	15	4	1544	1576	21	4	2460	2402
22	19	671	666	27	9	1199	1120	15	5	653	674	21	6	1849	1789
23	4	419	549	27	10	1773	1550	15	6	891	837	21	7	673	571
23	5	884	776	27	11	969	900	15	9	1173	1120	21	8	657	429
23	6	1369	1402	27	12	1817	1525	15	11	1157	1114	21	9	790	776
23	7	632	618	27	16	675	619	15	13	589	599	21	10	1036	953
23	8	631	539	27	17	1051	916	16	3	555	447	21	11	2068	1912
23	9	1087	971	27	19	837	756	16	4	661	453	21	12	524	499
23	10	541	686	27	21	501	449	16	5	667	649	21	13	1294	1281
23	11	640	679	28	-10	683	685	16	9	1168	1066	21	14	666	432
23	12	2552	2358	28	5	1123	1170	16	10	940	792	21	18	526	452
23	13	898	853	28	7	1511	1476	16	11	1206	966	22	3	566	462
23	14	762	669	28	9	953	890	16	12	601	583	22	4	965	913
24	4	374	361	28	11	4339	3794	17	3	534	638	22	5	2997	2829
24	5	586	568	28	13	4422	3794	17	4	2023	2138	22	6	1071	1114
24	6	1781	1915	28	15	2159	1894	17	5	428	337	22	7	1101	902
24	7	595	425	28	17	747	622	17	7	512	466	22	8	835	676
24	9	394	371	28	21	426	417	17	9	955	844	22	9	1398	1327
24	10	975	736	**H = 23****				17	11	920	974	22	10	1298	1314
24	11	1352	1193	6	4	619	483	17	12	532	500	22	11	1418	1167
24	13	1630	1479	7	4	441	497	17	13	735	776	22	12	1195	1091
24	14	759	735	7	5	351	393	17	14	556	455	22	13	616	524
24	15	593	663	8	3	1313	1365	17	15	701	586	22	14	575	499
24	16	631	481	8	4	391	272	17	17	933	874	22	15	1315	1181
25	4	940	753	8	7	376	438	18	3	1050	1258	22	16	506	148
25	5	337	236	9	4	1838	1787	18	5	439	368	22	19	531	565
25	6	398	346	9	6	540	519	18	7	1004	968	23	3	1389	1274
25	8	931	907	9	11	575	592	18	10	472	285	23	6	1048	1015
25	9	855	799	10	3	1018	1101	18	11	522	524	23	8	1130	1083
25	10	355	207	10	5	1041	1010	18	12	790	665	23	9	934	763
25	11	903	949	10	7	1085	944	18	14	643	544	23	10	1081	913
25	12	577	498	10	8	656	643	18	17	953	863	23	11	392	270
25	15	841	839	10	9	664	606	18	18	765	726	23	12	1525	1341
25	16	1133	1043	10	10	789	857	19	3	1270	1276	23	13	448	595
25	18	435	413	10	12	432	525	19	4	1533	1645	23	14	1377	1097
25	19	528	406	11	3	530	454	19	8	562	446	23	15	568	565
25	21	482	356	11	4	815	904	19	9	2342	2420	23	18	708	686
26	4	4679	4245	11	6	462	443	19	10	683	546	24	4	359	356



Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
	**H =	23****		28	17	1474	1115	16	4	847	801	21	10	1625	1607
24	5	449	453	28	19	472	293	16	6	621	568	21	11	864	975
24	7	525	478		**H =	24****		16	9	751	754	21	12	1523	1492
24	8	1251	1188	6	2	1516	1438	16	12	582	535	21	14	1036	862
24	9	1475	1435	6	4	821	706	17	2	990	1128	21	15	817	583
24	10	961	926	8	3	453	435	17	4	901	703	21	17	861	814
24	11	1417	1260	8	4	539	525	17	5	547	430	22	2	434	444
24	12	784	699	8	5	437	526	17	6	485	306	22	3	1261	1410
24	15	498	168	8	7	498	480	17	7	1115	1112	22	4	690	611
24	19	664	472	8	9	646	732	17	8	2032	2087	22	5	874	935
25	3	2713	2609	9	3	618	622	17	9	655	543	22	6	503	349
25	4	1053	1073	9	4	811	901	17	10	2012	1886	22	10	639	578
25	7	1730	1558	9	5	387	460	17	12	1179	1113	22	11	717	716
25	8	906	829	9	7	401	427	18	2	2406	2403	22	13	1015	956
25	9	1486	1325	9	8	717	731	18	3	457	335	22	15	1106	1092
25	10	686	623	9	10	657	634	18	4	2531	2522	22	17	696	655
25	11	1164	802	10	2	963	1103	18	6	1812	1754	22	18	477	584
25	12	709	692	10	7	400	336	18	7	1586	1534	22	19	578	370
25	13	522	540	10	11	586	438	18	8	506	454	23	2	498	439
25	14	1023	911	11	3	1736	1864	18	9	1733	1743	23	3	782	1001
25	15	1219	1191	11	5	561	681	18	10	582	435	23	4	463	500
25	19	435	342	11	11	481	519	18	12	736	843	23	5	601	726
26	3	1671	1635	11	12	716	710	18	13	898	949	23	7	1040	957
26	4	304	200	11	13	472	494	18	15	618	745	23	8	563	611
26	6	315	113	12	2	1390	1427	19	2	1017	754	23	9	825	774
26	7	1119	1007	12	3	724	755	19	3	6982	7122	23	10	1598	1596
26	8	1411	1229	12	4	869	875	19	5	2515	2380	23	12	605	498
26	10	3580	3156	12	8	422	294	19	6	497	449	23	13	853	939
26	11	1932	1889	12	9	865	808	19	7	1025	888	23	15	725	731
26	12	3722	3272	12	10	415	469	19	8	1097	1148	23	16	804	799
26	13	1790	1736	12	11	847	792	19	9	1070	1154	23	20	531	488
26	14	1463	1379	12	12	475	394	19	10	1349	1338	24	2	1467	1500
26	15	481	409	12	13	562	511	19	11	1619	1653	24	3	3147	3327
26	19	626	513	13	3	1081	1108	19	12	851	826	24	4	2561	2542
27	3	1383	1350	13	4	746	703	19	13	1418	1193	24	5	789	787
27	4	1436	1041	13	7	478	595	19	17	770	603	24	6	1746	1716
27	5	1269	1182	13	10	1005	995	20	2	758	598	24	7	534	556
27	6	1807	1542	13	11	638	617	20	3	1092	1017	24	9	569	642
27	7	409	208	13	12	540	555	20	4	1615	1493	24	10	551	525
27	8	3224	3006	14	2	1405	1612	20	5	669	669	24	11	1156	1053
27	9	948	867	14	4	593	643	20	6	1131	1077	24	13	695	598
27	10	2582	2353	14	6	606	756	20	7	756	666	24	14	877	700
27	11	880	741	14	8	1067	1133	20	8	2741	2466	24	18	516	373
27	12	827	620	14	9	572	413	20	9	507	404	25	3	1365	1073
27	15	1444	1239	14	10	1122	1155	20	10	2070	1791	25	4	291	120
27	16	506	452	14	12	541	684	20	11	1890	1797	25	5	758	456
27	17	959	964	14	15	713	742	20	12	631	564	25	7	1407	1260
27	18	1231	995	14	16	464	337	20	13	854	837	25	9	480	522
27	20	882	783	15	2	706	809	20	14	566	528	25	10	386	388
28	3	1828	2009	15	3	724	637	20	16	1045	835	25	11	443	487
28	5	4123	4057	15	4	593	528	20	18	956	975	25	13	1188	1001
28	7	2318	2158	15	7	735	809	20	19	691	648	25	14	615	532
28	8	339	0	15	9	802	765	21	2	1772	1646	25	16	1052	944
28	9	1638	1458	15	10	544	646	21	3	2323	2382	25	17	1185	963
28	11	2636	2534	15	11	779	651	21	4	1653	1802	26	2	5913	6197
28	13	2455	2367	15	12	1111	954	21	8	748	829	26	3	1069	1111
28	15	813	767	16	2	1917	1894	21	9	1401	1388	26	4	1056	1010

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 24****				10	8	855	792	17	15	847	828	22	6	599	599
26	5	1230	1035	10	9	506	374	17	16	584	514	22	9	2659	2589
26	6	498	574	10	10	490	436	17	17	534	502	22	10	717	764
26	7	1757	1535	11	1	546	614	18	1	2804	2866	22	11	903	876
26	9	2899	2574	11	2	521	425	18	2	393	390	22	12	722	679
26	11	1207	1197	11	3	994	1114	18	3	564	567	22	13	623	638
26	12	494	555	11	4	827	851	18	5	565	535	22	15	658	536
26	13	722	725	11	6	996	931	18	6	527	591	22	17	562	398
26	14	472	541	11	7	936	1097	18	10	1179	1100	23	1	1738	1956
26	15	525	369	11	8	728	651	18	11	533	321	23	2	2666	2194
26	16	1461	1283	11	9	1407	1503	18	12	1284	1254	23	3	1468	1678
26	18	816	809	11	10	749	787	18	14	628	582	23	4	887	879
26	19	842	897	11	11	563	689	18	15	1247	1089	23	8	1112	1057
27	2	1211	1241	12	1	1797	2027	18	17	901	897	23	9	388	440
27	3	778	839	12	2	769	791	18	18	508	491	23	10	691	512
27	4	310	161	12	3	969	931	19	1	1425	1630	23	11	969	778
27	5	446	356	12	4	420	516	19	2	608	451	23	12	1212	1211
27	6	968	830	12	5	609	624	19	4	1156	1210	23	13	541	490
27	7	1409	1299	12	8	798	738	19	5	1177	1143	23	16	1110	1014
27	8	1978	1786	12	10	434	292	19	6	706	732	23	18	652	549
27	9	2292	1959	12	12	570	589	19	7	1136	1174	24	1	488	464
27	11	1381	1215	12	14	541	590	19	9	2885	2744	24	3	388	72
27	12	1549	1304	13	1	526	440	19	10	725	583	24	4	439	87
27	14	2177	2122	13	2	1156	1180	19	11	2710	2434	24	5	758	762
27	16	962	939	13	3	623	550	19	13	1309	1262	24	6	1044	1017
27	17	1435	1303	13	5	557	478	19	14	668	623	24	8	531	497
27	18	766	712	13	6	830	825	19	16	1196	1094	24	9	1344	1361
27	19	617	648	13	8	663	616	19	18	494	388	24	10	402	181
27	20	955	961	13	9	844	891	20	1	3755	3765	24	11	441	407
28	3	1392	826	13	10	702	715	20	2	613	586	24	17	831	760
28	5	1086	660	13	11	1286	1348	20	3	2730	2518	25	1	360	762
28	7	617	573	13	13	923	996	20	4	1877	1856	25	3	2371	2414
28	9	4879	4426	14	2	1267	1381	20	5	1157	1181	25	4	842	799
28	11	4354	4077	14	4	614	553	20	6	1177	1235	25	5	358	66
28	13	2829	2628	14	6	863	762	20	8	1161	1261	25	7	1406	1340
28	15	851	802	14	9	482	556	20	11	783	837	25	8	563	539
28	19	978	1083	15	1	954	951	20	12	1446	1344	25	9	574	568
**H = 25****				15	2	949	897	20	13	935	924	25	10	917	790
6	4	441	465	15	3	901	1137	20	14	1791	1721	25	11	883	859
7	2	613	752	15	7	886	986	20	16	988	953	25	12	691	544
7	3	443	456	15	9	641	633	20	18	500	596	25	13	1622	1573
7	6	464	425	15	12	688	731	21	1	580	363	25	14	609	562
8	1	1436	1426	16	1	910	982	21	2	5228	5302	25	15	1251	1207
8	2	457	499	16	3	630	477	21	4	1619	1287	26	1	2566	2467
8	3	542	575	16	5	711	754	21	5	1472	1360	26	2	426	348
8	5	684	692	16	6	503	563	21	6	388	414	26	3	3952	3331
8	6	441	604	16	7	687	790	21	7	347	447	26	4	1233	871
9	2	1553	1552	16	8	1483	1499	21	8	913	1009	26	5	568	507
9	4	624	702	16	9	1276	1130	21	9	1840	1770	26	6	987	821
9	7	523	614	16	10	666	506	21	10	1016	896	26	7	747	829
9	9	482	581	16	11	718	603	21	11	1699	1602	26	8	2684	2573
10	1	1214	1211	16	14	824	920	21	16	524	595	26	9	795	699
10	2	480	388	16	15	564	554	21	19	587	601	26	10	3625	3216
10	3	960	1007	17	2	2697	2811	22	1	929	1020	26	12	2070	1999
10	5	1294	1331	17	3	805	933	22	2	1205	1251	26	18	473	455
10	6	512	440	17	4	1310	1281	22	3	1884	1559	26	20	551	524
10	7	991	1002	17	11	930	870	22	4	890	993	27	1	1256	1512

Table 45. Continued

K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL	K	L	FOBS	FCAL
**H = 25****				12	4	750	810	18	11	732	710	23	6	858	1089
27	3	246	133	12	7	499	521	18	13	1385	1374	23	10	1670	1535
27	4	1365	1562	12	9	936	967	19	0	1068	892	23	12	454	328
27	6	1177	1061	12	11	740	689	19	1	6481	6708	23	13	569	564
27	8	2053	1741	13	2	649	786	19	3	3163	3084	23	14	862	915
27	10	1639	1605	13	5	639	629	19	5	1259	1282	23	15	493	492
27	11	466	398	13	7	950	949	19	6	916	916	23	18	640	625
27	13	1171	1186	13	9	766	832	19	7	1258	1195	24	0	748	998
27	14	438	322	13	10	987	1044	19	8	1277	1166	24	1	708	720
27	15	1544	1448	14	0	2988	3211	19	10	969	1063	24	2	621	672
27	16	1078	1039	14	1	804	874	19	14	506	452	24	3	1001	1346
27	18	1013	981	14	2	1097	1248	19	15	790	600	24	6	718	659
28	1	15199	15285	14	3	480	516	20	0	3090	3240	24	9	548	396
28	3	7875	6641	14	4	620	457	20	3	403	327	24	10	999	851
28	5	364	168	14	6	689	720	20	4	1393	1357	24	11	712	748
28	7	2186	2138	14	8	827	789	20	6	837	753	24	14	688	540
28	9	1917	1821	14	10	498	634	20	7	1014	1072	24	17	683	585
28	11	2074	2009	14	13	866	955	20	8	2223	2271	25	1	581	209
28	13	459	435	14	14	602	560	20	9	1728	1743	25	2	867	837
28	15	1855	1701	15	0	662	648	20	10	1629	1730	25	3	1832	1394
28	17	1360	1304	15	1	1741	1931	20	11	1520	1485	25	4	706	708
**H = 26****				15	7	651	736	20	15	616	335	25	6	898	822
6	0	1310	1324	15	8	610	562	20	16	816	852	25	7	678	665
6	2	899	867	15	9	1078	1072	20	17	587	475	25	9	1214	1090
6	3	331	214	15	10	820	863	21	0	1708	2188	25	11	619	678
7	1	505	436	15	11	525	419	21	1	6314	6133	25	12	426	471
7	7	542	371	15	15	667	785	21	2	1393	1355	25	14	870	826
8	2	581	655	16	0	1165	1487	21	3	805	693	25	15	756	749
8	6	382	473	16	1	1171	1346	21	4	667	542	25	17	487	349
8	7	728	786	16	2	628	902	21	5	438	241	25	18	434	576
8	9	737	762	16	3	751	628	21	7	786	672	26	0	8586	8069
9	0	605	584	16	4	844	708	21	8	2155	2041	26	1	410	471
9	1	1189	1264	16	7	620	595	21	9	880	856	26	2	5995	5337
9	2	574	675	16	12	630	637	21	10	1849	1851	26	3	245	143
9	5	393	273	16	16	708	613	21	11	651	583	26	4	1796	1330
9	6	934	1008	17	1	703	633	21	12	962	929	26	5	791	832
9	8	1211	1245	17	2	1060	1300	21	13	903	984	26	6	763	675
9	10	665	756	17	3	391	376	21	15	1303	1306	26	7	808	810
10	0	746	821	17	4	495	594	21	17	782	787	26	9	698	612
10	5	711	655	17	5	647	656	22	0	3883	3763	26	10	356	212
10	7	519	553	17	6	708	1342	22	2	756	699	26	11	954	867
10	9	763	868	17	7	772	751	22	3	1774	2159	26	14	1298	1194
10	11	559	565	17	8	1702	1672	22	4	1319	1183	26	15	655	712
11	1	2016	2178	17	10	1527	1355	22	5	693	417	26	16	1271	1174
11	2	635	689	17	11	515	372	22	6	819	822	26	17	712	815
11	3	783	890	17	15	732	648	22	7	773	623	26	18	712	588
11	4	488	527	18	0	1533	1396	22	9	614	720	26	19	637	713
11	5	443	423	18	1	1209	1317	22	11	981	937	27	0	478	1142
11	6	456	506	18	2	1455	1449	22	13	695	781	27	1	380	59
11	9	562	616	18	3	995	1036	22	16	608	628	27	2	1605	1831
11	10	539	488	18	4	1695	1633	22	17	760	655	27	3	1339	1357
11	11	618	599	18	5	1557	1534	22	19	508	396	27	4	671	430
11	12	914	892	18	6	870	891	23	0	1175	1136	27	6	620	804
12	0	1114	1149	18	7	2700	2664	23	1	2010	1540	27	7	788	788
12	1	985	1065	18	8	946	1103	23	2	1716	1040	27	8	703	615
12	2	1135	1228	18	9	1555	1470	23	4	1732	1706	27	9	2361	2286
12	3	935	908	18	10	1042	1003	23	5	1278	1135	27	10	823	911

