IN-SITU RECOVERY PROCESS FLUIDS

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EXECUTIVE SUMMARY

The heavy oils produced from the Alberta oil sands contain cyclic organic compounds together with sulphur and nitrogen. Upon thermal treatment they have the potential to form carcinogenic, mutagenic, and toxic compounds. Recovery of oil by in-situ combustion processes, such as the Combination of Forward Combustion and Waterflood (COFCAW) process, may result in the formation of such biologically active compounds with generation dependent upon operating conditions.

The objective of the present research program is to evaluate produced oils and accompanying waters from in-situ combustion processes for possible biological activity. This evaluation is based on biological testing, using the Ames test for mutagenicity and the Microtox test for toxicity, and on the chemical analysis of oils and waters for the presence of known carcinogens. For comparison, oils produced by the less thermally rigorous steam injection process, as well as naturally occurring bitumen, and synthetic crude oil and other oils produced from the Athabasca and Peace River oil sands were examined.

Analysis of oils produced by in-situ combustion showed the presence of many carcinogenic and mutagenic compounds, among them the well known carcinogen benzo(a)pyrene (BaP). The BaP content of a mixture of bitumen, cracked oil, and diesel fuel produced by the COFCAW process from the Gregoire Lake pilot project contained 14 μg/g BaP. This compares with 1.5 μg/g in unaltered bitumen and 1 to 3 μg/g in most crude oils. Samples obtained from the Suffield Heavy Oil project which had not undergone rigorous thermal treatment contained from 1.5 to 7.5 μg/g benzo(a)pyrene and emulsion produced by steam injection from the Peace River Pilot project, operated by Shell Canada Resources Limited, contained 2.7 μg/g. An oil produced by dry retorting of the Athabasca oil sands contained 16 μg/g BaP. Oils produced from combustion tube experiments with Athabasca oil sand had a similar BaP content, 2.6 and 4.2 μg/g. Some tars and pitches, especially coal tars, may contain 10 to 100 times more BaP than crude petroleum. Refinery residuals, tars, and oils from Sarnia were found to contain 150 to

1050 μg/g. Benzo(a)pyrene is the best known of the carcinogens found in petroleum, but many other known or suspected carcinogens were found in greater quantities than BaP in the oils produced by in-situ combustion and dry retorting.

The assessment of any carcinogenic hazard associated with petroleum is difficult. Animal tests are expensive and time consuming; therefore, short term bio-assays for mutagenic properties such as the Ames test, together with chemical analysis, are employed. Positive results in the Ames test are not an absolute indicator of carcinogenic potential. Mutagenicity does not in all cases imply carcinogenicity; however, those polycyclic aromatic hydrocarbons which are carcinogenic are also mutagenic in the Ames test when appropriate enzymes are included.

Mutagenic activity was found with the Ames test in oils produced from the Gregoire Lake, Suffield, and Peace River in-situ pilot projects and in vacuum gas oil and pitch from the Peace River diluent recovery unit. The mutagenicity was less than predicted from the amount of carcinogenic aromatic compounds found by chemical analysis. The complex mixture of hydrocarbons which comprises these oils suppressed the activity of the carcinogens in the Ames test. Thus the Ames test was found to be an indicator of mutagenic activity but not a quantitative method for assessing the relative mutagenicity of oils. Synthetic crude oil produced from Athabasca bitumen displayed some mutagenic activity but, despite the presence of BaP, the bitumen itself did not.

Waters produced during in-situ recovery of oil by both steam stimulation and combustion processes were toxic to aquatic organisms as determined by the Microtox bioluminescence assay. EC_{50} values, the effective concentration of toxicant causing a 50% decrease in the light output of a photoluminescent bacteria, ranged from 0.30 to 11. The toxicity was caused partly by volatile organic compounds, primarily alkyl substituted benzenes, and partly by extractable organic compounds including phenols, organic acids, and hydrocarbons with no single class of compounds solely responsible for the observed toxicity. Wastewaters from the dry retorting process were more toxic than waters produced by in-situ combustion and contained many aromatic hydrocarbons and nitrogen compounds known to be biologically active.

The chemical analyses and limited biological testing carried out in this study detected no strong mutagenic or carcinogenic hazard associated with in-situ recovery of heavy oil by combustion and steam injection. The relative hazard is probably marginally greater than that associated with production of conventional light crude oils but far less than might be expected from coal liquefaction processes or from disposal of refinery residuals. The hazard associated with dry retorting is greater than that from in-situ recovery methods and care should be taken in the handling of both products and wastewaters from this process.

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ABSTRACT

Chemical analysis of oils, produced by in-situ combustion processes from the Athabasca oil sands, revealed many compounds known to be carcinogenic or mutagenic. Concentrations were low, up to 14 µg/g of benzo(a)pyrene (BaP). This compares with up to 7.5 µg/g BaP in soils produced by less rigorous thermal treatment from the Suffield block, 2.7 µg/g in oils produced by steam injection from the Peace River sands, and 16 µg/g in oils produced by the dry retorting of Athabasca sands. Some coal tars, pitches, and refinery residuals may contain more than 50 times these concentrations.

The Ames test was used as an indicator of mutagenic activity but could not be used as a quantitative means of comparing mutagenicity among oils. Activity was found in fractions of all the above oils but the activity was less than expected based upon the amounts of known carcinogens and mutagens found by chemical analysis.

Waters produced during both steam injection and in-situ combustion processes were toxic to aquatic organisms as determined by the Microtox bioluminescence assay. Toxicity was caused by dissolved aromatic hydrocarbons, phenols, organic acids, and nitrogen compounds. Waters from the dry retorting process were the most toxic of those tested.

On the basis of this limited testing, biological activity detected in oils produced by in-situ processes was slightly greater than that associated with normal crude oils but far less than might be expected from coal liquefaction products and refinery residuals.

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1. INTRODUCTION

With the gradual decline of Canada's easily recoverable conventional oil reserves, industry and government are increasingly looking toward more expensive sources of energy such as conventional oil offshore and in the Arctic, as well as conventional heavy oil reserves, and heavy oil sands.

The oil sands of northern Alberta represent one of the world's largest underutilized energy reserves, estimated to be from 950 or 1350 billion barrels of heavy oil (Mossop 1980; Nicholls and Luhning 1979). Commercial production, using surface mining and hot water extraction to separate the heavy oil, began in 1967 and production from the two large plants totals about 200,000 barrels per day. Unfortunately, the present commercial techniques can be economically applied to only about 8% of the in-place reserves, those which are covered with less than 50 m of overburden. Nevertheless, over 75 billion barrels of heavy oil could be recovered using the existing technology (based on 8% of the reserves).

Further development of large scale plants, using surface mining and hot water extraction, has been restricted by financial considerations. These plants require a very large capital investment (upwards of 10 billion dollars) and take five or more years to build. Worldwide political and financial uncertainties have made such large scale, long-term investments unattractive. Thus, there is a need for alternate methods of oil recovery which require less capital investment and which will recover oil from deeply buried sands.

In situ recovery methods may meet these criteria: projects can be initiated with a relatively small initial capital investment, can be brought into production more rapidly than large hot water extraction plants, can be expanded as demand for oil increases, and can be produced from sands not accessible by surface mining. Although many in situ recovery methods have been proposed, two basic methods, with several variations, have been extensively tested in pilot projects. The two methods are steam injection and in situ combustion. In both cases, a pattern of wells is drilled and communication between wells is established by fracturing the formation. Communication channels may be further established by injection of caustic solutions and emulsifiers. Steam is then injected, usually in a cyclic manner such as in the case of the "Huff and Puff" method where steam is injected at high pressure followed by depressurization of the formation to produce hot oil and water. In the COFCAW (Combination of Forward Combustion and Waterflood) a combustion zone is established in the formation, and water is injected to provide heat transfer and to drive the cracked and heated oil to production wells.

An alternative method is surface mining with recovery of the bitumen from the mined sands using a "dry" retorting process. Presumably a plant based on this process would be of smaller scale and consequently would require a smaller capital investment than the present hot water extraction plants.

Potential biological and environmental hazards have become major concerns in the development of large new energy technologies. Studies in the United States have focussed on the processing of coal and oil shales to produce liquid fuels. Epidemiological studies have shown an increased risk of cancer associated with these activities and fractions of the liquid fuels have produced cancer in test animals (Bridge and Henry 1928; Haagensen 1931; Heller 1930; Henry 1947; Sexton 1960). The cause of the carcinogenic activity is believed to be polycyclic aromatic hydrocarbons, heterocyclic compounds and other, as yet unidentified, compounds concentrated in the heavier fractions of the oil and residuals (Freudanthal et al. 1975; Kornreich 1976).

The opportunity for synthesis of hazardous chemicals exists whenever fossil fuels are subjected to severe conditions such as during pyrolysis, hydrogenation, or gasification. Such severe conditions exist in the combustion zone during recovery of oil from Alberta oil sands by the COFCAW process and, during dry retorting, with the Taciuk Processor in the UMATAC process. COFCAW-produced and UMATAC-produced oils may contain different types of compounds or greater amounts of some biologically active compounds than are normally found in crude oils. The composition of the produced oils varies according to the operating conditions of the process. Oils produced by steam injection undergo a far less rigorous thermal treatment than those produced by combustion and retorting methods.

In addition to carcinogenic substances, in situ processes are likely to produce many chemical compounds which are toxic to aquatic organisms. Some of these compounds will be dispersed or dissolved in formation waters in the vicinity of the production zone and, if not confined, may contaminate other subsurface waters. Such compounds could impart an unpleasant taste and odour to drinking waters; the possible health effects of long term exposure are not well understood. Waters co-produced with the oil or wastewaters from the "dry" retorting process may also present an environmental hazard if they are not properly confined or treated. Unfortunately, even under the most carefully controlled conditions, spills occasionally occur when large volumes of fluids are handled. Similarly, spills of produced oil or synthetic oil may find their way into surface waters or eventually into groundwaters. In addition to obvious toxic effects from chemical pollutants, the possibility of the compounds producing carcinogenic, mutagenic, or teratogenic effects whose expression may be divorced in time from the exposure(s) also requires consideration (Epler et al. 1978).

No simple, reliable, and inexpensive biological test presently exists for assessing the carcinogenicity of complex mixtures of compounds such as those recovered from the Alberta oil sands by in situ methods. Animal tests are expensive, time consuming, and not practical for determining the long-term effects of chronic exposure to low concentrations of carcinogens. Short-term, in vitro, bio-assays offer a number of advantages for the initial screening of samples for carcinogenic or mutagenic activity. They are quick, relatively inexpensive, reproducible, and sensitive. However, the extrapolation of results from short-term bioassays for mutagenicity to man is in question. Short-term tests point out potential mutagenic and carcinogenic chemicals and serve to order priorities for further testing. Biological screening tests such as the Ames Salmonella/microsome assay (Ames et al. 1975) have demonstrated their utility: (1) as indicators of potential long-term health effects such as mutagenesis and carcinogenesis; (2) as a means to direct the fractionation and identification of hazardous biological agents in complex mixtures; (3) as a measure of relative biological activity to be correlated with changes in process conditions; and (4) to establish priorities for further biological testing or chemical analysis (Waters 1979).

A second powerful tool is chemical analysis to quantitatively identify known carcinogenic or mutagenic compounds in complex hydrocarbon mixtures. Many hundreds of compounds, such as the well known carcinogen benzo(a)pyrene, can be identified down to the positional isomer level by this method. It is important that the specific isomers present be determined, since the biological activity of isomers of the same compound may vary greatly. Difficulties arise, however, in providing a biological interpretation of the chemical data. Of the hundreds of compounds which may be found, the carcinogenic or mutagenic properties of only a few may be known. Information is generally available only on pure chemicals and little is known about the behavior of mixtures of many carcinogenic and non-carcinogenic compounds.

A combination of biological testing and chemical analysis provides the best, although far from complete, means of assessing samples for mutagenic or carcinogenic hazard. Chemical fractionation may be required to simplify complex mixtures prior to biological testing, eliminating compounds which may be toxic to the test system and simplifying the chemical analysis.

Biological testing for acute toxicity in water systems is far better standardized than testing for mutagenesis or carcinogenesis. The 96 h fish test is widely used but is not universally applicable. For example, very few researchers have maintained constant concentrations of volatile components such as aromatic hydrocarbons for the duration of the test. Furthermore, the fish test is a measure of acute toxicity only, and there is little evidence that it is a measure of the effect of a compound on the ecosystem as a whole (Dickson 1982). The Microtox bioluminescence assay has been developed to partially overcome some of the limiting factors of the fish test. It is fast and precise, taking only a few minutes per assay, therefore minimizing loss of volatile compounds. Chemical analysis can be used to identify toxic organic compounds in the water and volatile organic compounds which may be lost during fish toxicity tests.

The objective of this research program is to evaluate produced fluids from the COFCAW in situ process and from other heavy oil recovery processes for possible toxic and carcinogenic properties. This evaluation is based on biological testing by the Microtox and Ames tests and on chemical analysis for the presence of known toxic and carcinogenic compounds.

Specific objectives of the program are:

1. To identify and quantitatively measure known carcinogenic and mutagenic compounds in oils and wastewaters produced during recovery of heavy oil by in-situ combustion (COFCAW process and SHOP project) and dry retorting processes (UMATAC);
2. For the purpose of comparison, to identify and quantitatively measure similar compounds in -
   (a) synthetic crude oil produced by the commercial surface mining method,
   (b) oil produced from the Athabasca and Peace River deposits by steam stimulation,
   (c) naturally occurring heavy oil from the Athabasca sands,
   (d) diesel fuel circulated downhole during heavy oil production, and
   (e) refinery tars and residuals;
3. To determine the mutagenic activity, based upon the Ames test, of oils produced by in-situ combustion recovery methods;
4. To determine the toxicity to aquatic organisms of waters coproduced with oil from the in-situ recovery pilots and dry retorting process;
5. To determine the toxicity of waters after contact with cracked hydrocarbon products from the oil sands; and
6. To compare results obtained from in-situ pilot projects with those from the more easily monitored combustion tube experiments carried out at the University of Calgary.

2. MATERIALS AND METHODS

2.1 SAMPLE DESCRIPTION

The fluids examined were primarily from the Suffield Heavy Oil Pilot (SHOP) project located about 50 km north of Suffield, Alberta, from the UMATAC dry retorting pilot plant located in Calgary, and from the Gregoire Lake pilot project located about 40 km southeast of Fort McMurray, Alberta. The Gregoire Lake pilot was operated by Amoco Canada Petroleum Company Limited on behalf of the Alberta Oil Sands Technology and Research Authority (AOSTRA), Amoco, Petro Canada, Sun Oil Company Limited, and Shell Canada Limited. The SHOP project is operated by Alberta Energy Company Limited (AEC) on behalf of its three partners: AOSTRA, Westcoast Petroleums Limited, and Muskateer Energy Limited (a wholly owned subsidiary of Dome Petroleum Limited). The UMATAC pilot plant is a joint AOSTRA-UMATAC Industrial Processes Ltd. project.

The SHOP project is designed to evaluate in-situ combustion as a means of increasing heavy oil recovery. About 69,000,000 m^3 (430,000,000 barrels) of viscous heavy oil have been found in the Suffield Military Block but only a small proportion of this can be recovered by conventional primary and secondary recovery methods. The project consists of a central injection well and four production wells located 140 m apart and 100 m from the injection well. Three observation wells are located within the square of production wells. Samples of produced oil and water were taken in 1983 and 1984.

The Gregoire Lake pilot project was designed for the extraction of deep oil from Alberta's oil sands by the COFCAW in-situ process. Initially, the project was to consist of nine injection wells and sixteen production wells with a spacing of one production well per hectare. Subsequently, the spacing of wells was modified by the addition of satellite wells located in each case about 8 m from the production wells in the direction of the injection wells. Not all wells within the pilot project produced by the COFCAW process, some produced by steam stimulation.

Communication among injection and neighbouring production wells was not always well established or defined; thus, produced waters may have been derived directly from the COFCAW process, from a combination of the COFCAW process and steam stimulation, or from steam stimulation alone. Some original connate water may also have been produced. Diesel fuel was circulated downhole to prevent blockage with heavy bitumen. Produced oil may consist of a mixture of raw bitumen, bitumen heated by steam injection, hydrocarbons generated by in situ combustion and diesel fuel.

Fluids from the Gregoire Lake pilot project were sampled on February 19, March 19, May 14, and June 10 1981 (Table 1). A total of five wells was sampled with produced water and oil-water emulsion collected in 20 L glass containers. Smaller samples for Microtox testing, total organic carbon analysis, and analysis of volatile components were collected in 50 mL culture tubes tightly closed with teflon-lined screw caps. Not all wells were producing during each sampling period. Diesel fuel, which is circulated downhole to prevent blockages, was sampled prior to injection, and groundwater which is injected during the COFCAW operations was also sampled. Historic samples of oils and emulsions were also obtained. These included tubing samples taken from well GP26 June 10, June 24, and September 27 1980 and from well GP29 on July 12 1978.

The well designated GP26, when sampled in May, provided a good example of COFCAW-produced fluids. GP19, sampled in May and June, was produced primarily by steam stimulation. For comparison purposes, produced fluids and cracked products from the AOSTRA-Shell pilot study at Peace River were also examined as were commercial synthetic crude oil from the Athabasca oil sands, Athabasca bitumen, and conventional crude oils. Samples of produced emulsion were collected from well #44 of the Peace River pilot project on July 13 1982. Also sampled were the diluent, top oil, pitch, and vacuum gas oil from the diluent recovery unit.

Refinery residuals and tars are known to contain high concentrations of polycyclic aromatic hydrocarbons. To assist in putting the in-situ combustion results into perspective, five types of samples ranging in viscosity from gas oil to fractionator bottoms were obtained. A list of all samples is contained in Table 1.

Table 1. List of samples obtained for this study.

1. Samples taken from the Suffield Heavy Oil Pilot Project.

Base sample - produced prior to initiation of in-situ combustion or steam injection.

Sampling date - January 27 1983

- treater water
- oil from treater
- defoamer chemical
- de-emulsifier chemical
- biocide

Sampling date - February 2 1983

- Well P1 oil and water
- Well P2 oil and water
- Well P3 oil and water
- Well P4 oil and water

Sampling date - May 12 1983

- treater water
- treater oil
- Well P1 wellhead oil
- Well P2 wellhead oil
- Well P3 wellhead oil
- Well P4 wellhead oil

Sampling date - February 29 1984

- treater water
- oil from treater
- Well P1 wellhead oil
- Well P2 wellhead oil
- Well P3 wellhead oil

2. Samples taken from the Gregoire Lake pilot study.

2.1 Water Samples

GP-20 (Feb) GP-20 (Mar)	Produced water; combination of treated water, raw water and stimulated water (100^{o}C)
GP-21 (Feb) GP-21 (Mar)	Produced water; combination of raw water and stimulated water (100^{o}C)
GP-21 (Jun)	COFCAW-produced water

continued...

Table 1. Continued.

GP-26 (Feb)	Water produced in combustion process
GP-26 (Mar)	
GP-26 (May)	
GP-31 (Feb)	Produced waters from steam stimulation
GP-31 (Jun)	
GP-19 (May)	Produced waters from steam stimulation
GP-19 (Jun)	
Groundwater (Feb)	Groundwater used for injection of samples
2.2 Oil Samples	
GP-31 (Feb)	Steam produced bitumen
GP-31 (Mar)	
GP-19 (May)	Steam produced bitumen
GP-19 (Jun)	
GP-26 (May)	COFCAW-produced bitumen
GP-21 (Jun)	Steam produced bitumen
GP-26 (Jun 1980)	Historic sample, COFCAW-produced 80-6-10
GP-26 (Jun 1980)	Historic sample, COFCAW-produced 80-6-24
GP-26 (Sep 1980)	Historic sample, COFCAW-produced 80-9-27
GP-29 (Jul 1978)	Historic sample, 78-7-12
Tank sample, T. (Feb)	Cumulative oil sample from top of storage tank
Tank sample, M. (Feb)	Cumulative oil sample from middle of storage tank
Tank sample, B. (Feb)	Cumulative oil sample from bottom of storage tank
Tank sample, T. (Jun)	Cumulative oil sample from top of storage tank
2.3 Diesel Fuel	
Diesel fuel, A.	Diesel used to circulate downhole, no inhibitors
Diesel fuel, B.	Diesel used to circulate downhole, inhibitors added

3. <u>Refinery Samples</u>.
November 1982

- steam cracker gas oil
- catalytic cracker heavy cycle oil
- catalytic cracker fractionator bottoms
- fluid coker heavy gas oil

continued...

Table 1. Continued.

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4. Peace River Samples.
July 1982

- oil-water emulsion
- diluent
- top oil
- pitch
- vacuum gas oil

5. UMATAC Samples.
October 1982

- off gas condensate
- day tank product
- overhead oil
- sidedraw oil
- preheat steam vent oil
- bottoms
- scrubber settling tank underflow
- preheat vent water
- overhead vent water
- oil sand feedstock
- tailings
- hydrocarbon cyclone solids
- flue cyclone solids

September 11 1984
- preheat vent water
- overhead vent water

September 26 1984
- overhead vent water (preserved)

September 27 1984
- overhead vent water

October 12 1984
- overhead vent water
- preheat vent water

October 14 1984
- overhead vent water

November 8 1984
- overhead vent water (preserved)
- preheat vent water (preserved)

Continued ...

Table 1. Concluded.

November 21 1984
- preheat vent water
- overhead vent water

6. Combustion Tube Experiments.

February 1983
- 159-2 oil
- 159-6 oil
- 159-11 oil
- 159-13 oil
- 159-14 oil

October 1983
- 168-1 oil-water emulsion
- 168-5 oil-water emulsion
- 168-9 water
- 168-12 water

November 1983
- 169-6 water
- 169-8 water
- 169-9 water
- 169-11 water
- 169-13 water
- 169-15 water
- 169-18 water
- 169-20 water

7. Other Samples.

- Lloydminster heavy crude oil
- Athabasca bitumen
- Pembina light crude oil

The UMATAC pilot project utilizes the Taciuk Processor to separate bitumen from oil sands by retorting. The process combines retorting of bitumen from the sand with burning of the deposited coke within the same vessel. The system is described as "dry" because no water or steam is added; nevertheless, water which is normally present in mined sand is produced. Several product and wastewater streams were sampled.

2.2 EXTRACTION AND FRACTIONATION OF ORGANIC COMPOUNDS

2.2.1 Water Samples

Water samples were extracted in the 20 L bottles used for sample collection. The extraction and separation scheme is shown in Figure 1. Similar schemes have been used in this and other laboratories for the fractionation of samples prior to chemical analysis or mutagenicity testing (Rubin et al., 1976; Strosher and Peake, 1978).

The neutral and acidic organic components were extracted by first acidifying the sample to pH 2 with concentrated hydrochloric acid and then mixing for a period of 6 to 18 h with 200 mL of benzene using a magnetic stirrer. After allowing the aqueous and solvent phases to separate, the benzene and any emulsion were removed. Four to five extractions were made with 200 mL of benzene per extraction.

Following extraction of the acidic and neutral compounds, the water sample was adjusted to pH 11 with sodium hydroxide, and the basic organic components were extracted with benzene. Two to three extractions were carried out in the same manner as for the acidic compounds.

The water was neutralized with hydrochloric acid and any amphoteric compounds were extracted two to three times with benzene.

Emulsions formed during the extraction process were broken by centrifugation or by freezing. The combined benzene extracts for each pH were concentrated under vacuum using a rotary evaporator at a temperature of 25°C.

The acidic extract was then fractionated into neutral, acidic, and asphaltene components. Acidic components were removed from the benzene extract by extraction with 5% sodium hydroxide. The remaining benzene layer containing neutral components was washed with double

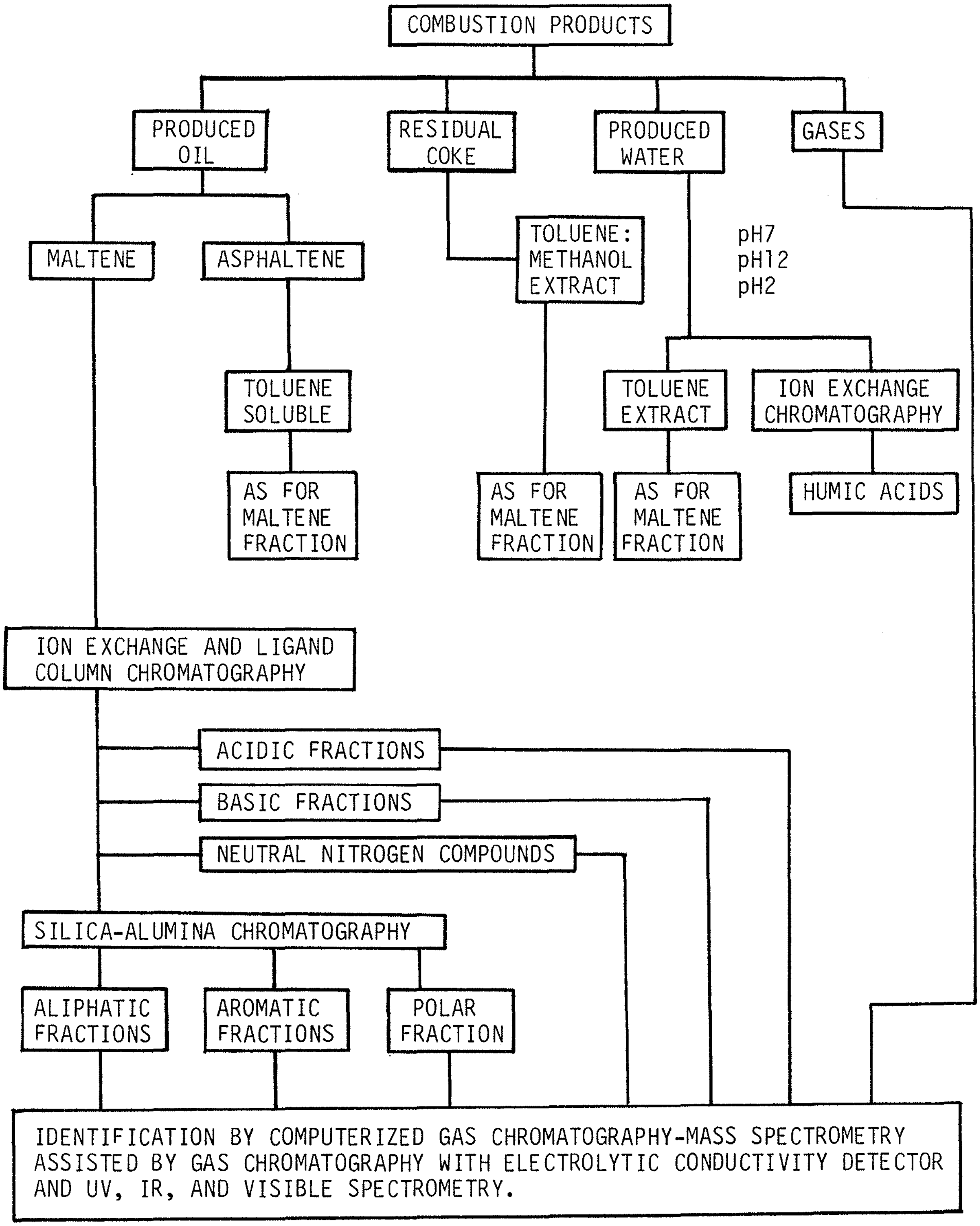

Figure 1. Analytical scheme for the separation and identification of organic compounds.

distilled water and reduced to near dryness. The residue was dispersed in pentane, allowed to stand overnight, and the asphaltenes separated by filtration. Neutral components remained in the pentane supernatant.

Acidic components dissolved in the sodium hydroxide solution were recovered by adjusting the aqueous pH solution to 2 and extracting with benzene.

2.2.2 Oil Samples

2.2.2.1 Fractionation with ion exchange resins. Asphaltenes were separated from the oil by dispersing the oil in pentane and allowing the asphaltenes to precipitate overnight. The asphaltenes were filtered from the sample, washed, dried, and weighed.

Twelve to 15 g of pentane soluble oil in 150 mL of pentane was passed through 40 g of Amberlyst A26 anion exchange resin in a 1 x 100 cm water-jacketed column. This column is part of an extraction apparatus which allows unreacted material to be removed from the resin by continuous extraction with 200 mL of hot pentane. Weaker acids were removed from the anion exchange resin by continuous extraction with 200 mL of benzene. The resin was then removed from the column and stronger acids removed by soxhlet extraction with 60% benzene-40% methanol. Any remaining acids were removed by extraction with methanol saturated with carbon dioxide.

The neutral and basic components which passed through the anion exchange resin were separated on a column of Amberlyst 15 cation exchange resin. Neutral compounds passed through the resin and any unreacted material was removed by refluxing with 200 mL of pentane. Bases were removed from the cation exchange resin in four stages, refluxing with 250 mL of benzene, 250 mL of 60% benzene-40% methanol, 250 mL of 55% benzene-37% methanol-8% isopropylamine, and 250 mL methanol.

The acids, bases, and neutral components were then subjected to further fractionation or analysed directly by combined gas chromatography-mass spectrometry and their mutagenicity determined by the Ames test.

2.2.2.2 Separation of nitrogen compounds on ferric chloride. Neutral nitrogen compounds were separated from the neutral nitrogen fraction remaining after chromatography of oil on ion exchange resins (Jewell et al. 1972). The neutral nitrogen compounds were complexed with ferric chloride by slow percolation through a column of ferric chloride supported on clay. Unreacted material was removed from the column with 10 volumes of pentane. The "neutral nitrogen" compounds were removed by eluting with 40 volumes of 1,2-dichlorethane. The neutral nitrogen fraction was then analysed by combined gas chromatography-mass spectrometry and the mutagenicity determined by the Ames test.

2.2.2.3 Separation by acid/base extraction. As an alternative to separation on resins (2.2.2.1), oils were separated into acids, bases, and neutral components with acid/base extractions. About 1 g of oil, freed of asphaltenes, was dissolved in 150 mL of diethyl ether. Basic compounds were extracted with 100 mL of 1N hydrochloric acid and acidic compounds with 100 mL of 1N sodium hydroxide. After backwashing with ether to remove any entrained hydrocarbons, the pH of the hydrochloric acid solution was adjusted to 11 with 12N sodium hydroxide and the basic compounds extracted with diethyl ether. The sodium hydroxide extract of the oil was also backwashed to remove any dispersed oil. Weak acids were separated by adjusting the pH of the sodium hydroxide extract to 6.5 with concentrated hydrochloric acid and partitioned with diethyl ether. Strong acids were extracted with diethyl ether after adjusting the sodium hydroxide extract to pH 1.5 with concentrated hydrochloric acid. The acids and bases were analysed by gas chromatography and tested for mutagenicity with the Ames test.

2.2.3 Separation of Aromatic Compounds from Oil-Water Emulsions.

Oil was separated from oil-water-clay mineral emulsions by repeated extraction with cyclohexane and centrifugation. The weight of extracted oil was determined by reducing an aliquot of the cyclohexane extract to near constant weight by rotary evaporation.

Aromatic hydrocarbons and compounds of similar polarity were extracted from the cyclohexane-oil mixture by shaking vigorously with an equal volume of 90% dimethylformamide-10% water (Grimmer and

Hildebrandt 1972). The resulting emulsion was centrifuged and the cyclohexane layer removed. The aqueous emulsion was repeatedly shaken with cyclohexane and centrifuged until the emulsion was broken and an aqueous dimethylformamide (DMF) phase was recovered. The DMF, containing the aromatic hydrocarbons, was filtered to remove any oil droplets.

The above procedure was repeated three times and the DMF extracts combined. The aromatic hydrocarbons were then transferred from the DMF solution into cyclohexane by adding 5 volumes of water saturated with sodium chloride and extracting three times with cyclohexane.

After removal of most of the cyclohexane by rotary evaporator, the crude aromatic fraction was chromatographed on a 20 x 120 mm column of deactivated Woelm 101 alumina (Adamek 1972). The aromatic compounds were eluted with 400 mL of toluene, leaving more polar compounds adsorbed in the alumina. The aromatic fraction was then rechromatographed on a 1 x 20 cm column of Woelm 101 alumina activated 16 hours at 300°C. Two hundred mL of toluene was used to elute the aromatics which were collected in 29 fractions ranging from 3 to 10 mL in volume. Fractions were then examined by synchronous fluorescence spectroscopy, analysed by combined gas chromatography-mass spectrometry, and their mutagenicity determined in the Ames test.

2.3 CHEMICAL ANALYSIS OF PRODUCED WATERS

2.3.1 Total Organic Carbon (TOC)

Samples collected in 50 mL culture tubes were analysed for total organic carbon with a Dohrmann Envirotech carbon analyzer. The sample was shaken prior to analysis and therefore the TOC values represent both dissolved organic compounds and compounds associated with suspended matter. The method also gives a value for "volatile organic carbon" representing compounds boiling up to about 150°C.

2.3.2 Volatile Organic Compounds

Volatile organic compounds were analysed by combined gas chromatography-mass spectrometry after concentration by a modified purge and trap method (USEPA 1977). From 0.5 to 5.0 mL of sample was placed in a 13 x 100 mm culture tube and the volume brought to 5 mL by the addition of distilled water as necessary. The tube was heated to 45°C in a water bath and helium passed through the sample via a length of fused silica capillary tubing at the rate of 50 mL per minute. The purged hydrocarbons were trapped in a 40 x 10 mm glass column filled with Tenax GC resin. The hydrocarbons were removed from the Tenax resin by heating to about 250°C with helium flowing at 50 mL per minute and were trapped in a length of fused silica tubing at liquid nitrogen temperature. The hydrocarbons were then flashed into the injection port of a combined gas chromatograph mass spectrometer (GC-MS) and analysed. The GC-MS system used was a Finnegan model 4021 equipped with an INCOS data system, a Wanco 10 megabite disc drive, and a Perkin Elmer 9 track tape drive. Separation was achieved on a 30 m by 0.25 mm fused silica column coated with SE54 having 107 000 actual plates. The fused silica contains few active sites, thereby allowing high resolution of acids and bases as well as neutral compounds. GC-MS operating conditions are listed in Table 2. Tentative identifications of the purged hydrocarbons were based on computer comparisons with mass spectra contained in the United States Environmental Protection Agency library of 26 000 compounds.

2.3.3 Extractable Organic Compounds

Acidic, basic, and neutral organic fractions, separated from water and oil samples as described in Section 2.2, were analysed by combined gas chromatograph-mass spectrometry (GC-MS). GC-MS operating conditions are listed in Table 3. Identification of compounds was based on: (1) computer comparisons of mass spectra with those of the United States Environmental Protection Agency library; (2) gas chromatograph retention times as compared with standard compounds; and (3) published mass spectra and gas chromatographic data. Quantification was based on internal standards of deuterated anthracene, chrysene, and benzo(a)pyrene. Separate samples were fractionated for chemical analysis and biological testing, with the deuterated standards being added prior to extraction and fractionation for those samples which were to undergo chemical analysis.

Table 2. Gas chromatograph-mass spectrometer conditions for analysis of volatile compounds.

Gas Chromatograph	
Column	30 m x 0.25 mm fused silica coated with SE54 (J. and W. Scientific)
Carrier gas	helium at 15 psi
Temperature program	15°C for 10 minutes, 15° to 70°C at 25° per minute, 70° to 180°C at 4° per minute, hold at 180°C for 30 minutes.
Injection port temperature	200°C
Transfer line temperature	200°C
Mass Spectrometer	
Ionizing voltage	50 ev
Mass range	45 to 250 amu
Scan rate	full range each 0.5 seconds
Manifold temperature	100°C
Manifold pressure	5×10^{-7} torr

Table 3. Gas chromatograph-mass spectrometer conditions for analysis of extracted compounds.

Gas Chromatograph	
Column	30 m x 0.25 mm fused silica coated with SE54 (J. and W. Scientific)
Carrier gas	Helium at 15 psi
Temperature program	40°C for 1 minute, 40 to 100°C at 40° per minute, 100 to 300°C at 4° per minute, hold at 300°C for 20 minutes.
Injection port temperature	300°C
Transfer line temperature	300°C
Mass Spectrometer	
Ionizing voltage	50 ev
Mass range	45 to 425 amu
Scan rate	full range once per second
Manifold temperatures	100°C
Manifold pressure	1.1×10^{-6} torr

Aromatic hydrocarbon fractions were examined by synchronous excitation-emission spectrofluorometry as well as by GC-MS. The instrument used was a Turner model 210 operated with 23 nm between the excitation and emission wavelength and scanning from an excitation of 275 to 550 nm. In this mode 2-ring aromatic compounds give emissions in the 290-330 nm range, 3 and 4-ring compounds emit from 330 to 390 nm and compounds with 5 or more rings emit at wavelengths higher than 390 nm.

2.4 BIOLOGICAL TESTING

2.4.1 Microtox Toxicity Test of Waters

The Microtox system was used to test the produced waters and waters contaminated with cracked oil products for toxicity to aquatic organisms. Produced water samples were tested: (1) as received; (2) after purging with helium to remove volatile organic components as described in 2.3.2; and (3) after extraction to remove acidic, basic, and neutral compounds. Waters contaminated with cracked oils were tested before and after removal of volatile compounds.

In the past, time-consuming static or flow-through bio-assays were used to monitor for toxic components in water, but the Microtox method, using luminescent bacteria and requiring small quantities of toxicant, produces results in less than one hour.

The Microtox toxicity system is a true bio-assay based on the response of live luminescent microorganisms. The reagent organism used is a marine bacterium closely resembling *Photobacterium phosphoreum*, selected because of its response to a wide spectrum of toxicants. The metabolic processes of the cells is a reflection of their state of health and is influenced by low concentrations of toxicants which cause a decrease in their light output.

This system uses the EC_{50} designation as an expression of toxicity. The EC_{50} value is the effective concentration of toxicant or effluent causing a 50% decrease in the light output of the bacteria under defined conditions of time and temperature.

Previous work compared Microtox EC_{50} data for a series of pure compounds, including benzene, phenol and trinitrotoluene (Bulich et al. 1981; Qureshi et al. 1982; Chang et al. 1981). The data indicate good general agreement between the Microtox bio-assay and fish bio-assay and Bulich concluded that five minute Microtox EC_{50} values were comparable with the fish 24 to 96 h data. In the same study, over 50 complex effluent samples were assayed with Microtox and simultaneously assayed using standard fish testing procedures. Good general agreement was shown between tests but no attempt was made to account for differences in test conditions such as temperature, pH, water hardness, and other study factors.

Studies conducted by Lebsack et al. (1981) on fossil-fuel process waters and some phenolic components indicate that the correlation between the Microtox and fish bio-assay was indeed as good as the correlation between LC_{50}'s of two fish species. Therefore, the Microtox system is an efficient and fast method of determining the presence of potentially harmful components in process waters being returned to the environment. The system does have limitations, and such parameters as pH, nutrient load, and salinity can have an effect and must be considered in the final analysis.

The Microtox reagent is composed of freeze-dried cells of luminescent bacterium, commonly found in marine environments and harmless to man. Being of marine origin, these bacteria have a minimal requirement of osmotic protection provided by addition of NaCl to the test solution. The bacteria display good light stability in the presence of 2% NaCl, although salinities between 0.5% and 4% can be used, provided that all components of the test are adjusted to the same salinity.

Samples with high nutrients may stimulate growth of the bacteria, causing a light increase. This was overcome by using potassium phosphate as the blank and as a growth medium for the bacteria. Highly coloured samples may cause a non-specific reduction in bacterial light output in the normal Microtox test. A colour correction procedure has been developed which uses a special two-chambered sample cuvette to provide a measure of light adsorption due to colour of the sample.

Lyophilized luminescent bacteria were hydrated, before each test, with 1.0 mL of reconstituting solution precooled to $3.0^{\circ} \pm 1^{\circ}C$. Five to seven pairs of cuvettes were placed in an incubator block controlled at $15^{\circ}C$. To one cuvette of each pair, the test cuvette, was added 500 μL of Microtox diluent, which is purified water containing 2% NaCl. The second cuvette of each set received 1.0 mL of an appropriate sample dilution with the exception of one cuvette which contained Microtox diluent. This cuvette served as a blank.

After the test cuvettes were cooled to 15^{0}C, 10 μL of rehydrated bacteria was added to each of the cells and allowed to stabilize for 15 minutes. Five hundred microlitres of the sample and 500 μL of the blank solutions were transferred to the appropriate cell suspension. Initial light readings were then recorded for each cell suspension. Light readings were recorded for each cell after 5 minute and 15 minute reaction periods.

The blank was used to correct for time-dependent drift in light output. Those cuvettes which had been challenged with a toxic sample displayed a decrease in light level. Comparison of light decrease versus concentration of sample was used to determine an EC_{50} value.

2.4.2 Ames Mutagenicity Test of Fractionated Oil and Water Samples

Fractions separated from waters and oils as described in 2.2 were tested for mutagenic activity using the Salmonella mammalian-microsome mutagenicity test (Ames et al. 1975).

An aliquot of the fractionated sample was reduced to incipient dryness by rotary evaporation and evaporation under a stream of nitrogen gas. The residue was weighed and dissolved in dimethylsulphoxide (DMSO). Extracts in DMSO were tested and assayed for mutagenic activity using the spot test and quantitative plate test in which the sample, bacteria, and mammalian enzymes were incorporated in an overlay of molten agar on plates containing minimal glucose agar medium (1.5% Difco Bacto-agar, 0.2% glucose, 1.05% K_2HPO_4, 0.45% KH_2PO_4, 1.0% $(NH_4)_2SO_4$, and 0.1% $(NH_4)_2SO_4$, and 0.01% $MgSO_4 \cdot 7H_2O$).

Bacterial strains received from Dr. Bruce Ames, University of California (Berkeley), were checked for histidine requirements, deep rough character, ampicillin resistance, uv-sensitivity, and spontaneous reversion rate prior to storage as frozen cultures (-80^{0}C). Initial testing with strains TA98 and TA100 showed that TA98 gave the most consistant and reliable results; therefore, TA98 was selected for routine testing of fractions. This strain detects frame-shift mutations including those which are enhanced by the presence of an R-factor. The bacteria were grown overnight to saturation in a Penassay broth culture to which was added 0.1 mL of aqueous 0.2% ampicillin per 20 mL of broth (Parker 1979). The use of ampicillin in the growth of strains which carry the R-factor (TA98 and TA100) inhibited the growth of cells which had lost the R-factor and so ensured a near 100% R^+ cell population in the saturated culture.

Microsomal enzymes were obtained by homogenizing livers excised from rats injected 5 days previously with PCB (Aroclor 1254). Aliquots of the liver homogenate (termed S-9) were stored at -80°C until used. The optimum amount of S-9 per plate was determined with benzo(a)pyrene and sample extracts.

During routine testing, positive and negative controls were used to monitor consistency in both enzyme activity and bacterial properties.

The linear dose range was obtained by initially testing samples at a wide range of concentrations. Having determined the region of linearity (i.e., region of minimal toxicity), a narrower range of concentrations was used to determine the activity quantitatively. The slope of the line represents the mutagenic activity of the sample expressed in numbers of revertants per microlitre of extract in DMSO. From this can be calculated the number of revertants per litre of water sample or per gram of oil.

3. RESULTS AND DISCUSSION

3.1 CHEMICAL ANALYSIS OF PRODUCED WATERS AND WASTEWATERS

3.1.1 Acidity

The pH values of coproduced waters and plant wastewaters are listed in Table 4. The most acidic samples were obtained from the combustion tube experiments with pH values as low as 1.6. Waters produced from the Gregoire Lake well GP-26 in May, during production from the combustion zone were also low, at pH 2.7, and waters produced by the UMATAC process such as the preheat vent water produced in October of 1982 were also low, at pH 2.5.

Low pH values are typical of waters produced from fire-flood operations or waters from oil sands which have undergone pyrolysis. Other Gregoire Lake water samples had pH values in the range of 6.5 to 8.7, indicative of production by steam stimulation or of mixed production rather than waters from the COFCAW process. The pH of treater waters from the SHOP project was in the range 7.8 to 8.15. These waters may not be representative of wellhead production but if this is the case, they have not been produced from the combustion zone. Water from the Peace River pilot, well 44, had a pH of 6.4.

3.1.2 Organic Carbon Content of Produced Waters and Wastewaters.

The non-volatile organic carbon content of the samples ranged greatly. For the Gregoire Lake samples, the range was from 74 ppm for a sample collected from well GP-20 in March, to 1850 ppm for a sample collected from well GP-31 in February when GP-31 was producing by steam stimulation.

Although the sample of GP-31 water was collected from the test separator, it contained quantities of suspended clay minerals with which oil was associated. Most samples had organic carbon contents of 100 to 300 ppm with the May sample from GP-26 obtained during the fire-flood operations, containing a relatively high 481 ppm.

Table 4. Acidity and carbon content of water samples.

Sample	pH	Volatile Carbon (ppm)	Organic Carbon (ppm) (excluding volatiles)
SHOP			
Treater water (Jan 1983)	8.15	75	153
Treater water (Feb 1983)	7.8	171	340
Treater water (Feb 1984)	8.0	--	--
GREGOIRE LAKE			
GP-20 (Feb 1981)	6.80	21	116
GP-20 (Mar 1981)	7.10	10	74
GP-21 (Feb 1981)	7.60	11	96
GP-21 (Mar 1981)	8.65	21	103
GP-21 (Jun 1981)	8.55	38	202
GP-26 (Feb 1981)	5.60	21	160
GP-26 (Mar 1981)	6.95	33	170
GP-26 (May 1981)	2.70	136	481
GP-31 (Feb 1981)	7.15	242	1850
GP-31 (Mar 1981)	8.15	82	281
GP-19 (May 1981)	6.70	25	226
GP-19 (Jun 1981)	6.55	26	235
PEACE RIVER			
Well 44 (Jul 1982)	6.4	59	376
UMATAC			
Overhead vent (Oct 13 1982)	4.4	90	4828
Preheat vent (Oct 13 1982)	2.5	22	639
Scrubber tank (Oct 13 1982)	2.8	0	68

continued...

Table 4. Concluded.

Sample	pH	Volatile Carbon (ppm)	Organic Carbon (ppm) (excluding volatiles)
Preheat vent (Sep 11 1984)	7.1	4	150
Overhead vent (Sep 11 1984)	5.2	77	9210
Overhead vent (Sep 26 1984)	--	--	4190
Overhead vent (Sep 27 1984)	--	--	5350
Preheat vent (Oct 12 1984)	3.2	0	1340
Overhead vent (Oct 12 1984)	4.2	260	5510
Overhead vent (Oct 14 1984)	3.6	1240	8510
Preheat vent (Nov 8 1984)	--	15	131
Overhead vent (Nov 8 1984)	--	588	3970
Preheat vent (Nov 21 1984)	3.5	0	124
Overhead vent (Nov 21 1984)	4.4	147	5570
<u>COMBUSTION TUBE</u>			
168-9 (Oct 1983)	8.1	55	1035
168-12 (Oct 1983)	8.3	110	1090
169-6 (Nov 1983)	5.2	61	1250
169-8 (Nov 1983)	4.0	41	1270
169-9 (Nov 1983)	4.1	100	1470
169-11 (Nov 1983)	2.6	295	4515
169-13 (Nov 1983)	2.2	180	3880
169-15 (Nov 1983)	1.6	47	6340
169-18 (Nov 1983)	1.7	353	5215
169-20 (Nov 1983)	1.7	227	3910

The volatile organic carbon values for the Gregoire Lake samples ranged from 10 to 242 ppm. The 242 ppm value was obtained in the February GP-31 sample which contained considerable amounts of suspended clay minerals. The volatile organic carbon content of the COFCAW-produced water GP-26 collected in May was high at 136 ppm as compared with values of from 20 to 40 ppm for most samples. The volatile organic carbon content of GP-26 (May) was 28% of the total organic carbon whereas in other samples the volatile carbon generally represented less than 20% of the total organic carbon. Thus, it appears that cracked hydrocarbons produced by the COFCAW process had been dispersed or dissolved in the waters produced from GP-26 in May.

Only three water samples from the SHOP project were analysed for carbon content. Values for volatile carbon and non-volatile organic carbon fell within the range found for the Gregoire Lake samples.

The combustion tube experiments produced waters containing large amounts of dissolved or dispersed organic carbon. Non-volatile organic carbon contents ranged from 1035 to 6340 ppm and the volatile carbon from 41 to 353 ppm. These samples had been filtered through a Whatman number 1 filter paper.

The UMATAC process generated wastewaters with as much as 9210 ppm non-volatile organic carbon and up to 1240 ppm volatile carbon. These high values were found in the overhead vent condensate. The preheat vent condensate contained less organic carbon, from 124 to 1340 ppm non-volatile organic carbon and from 0 to 22 ppm volatile carbon.

3.1.3 Gross Extractable Components

The 20 L water samples were extracted in the glass bottles in which they were collected as described in 2.2.1. The resulting material obtained under acidic extraction conditions was further fractionated into acidic and neutral compounds, and the asphaltenes in the neutral material were determined. The results, giving a breakdown of the gross composition of the extractable organic material from the produced waters, are shown in Table 5.

Table 5. Composition of organic material extracted from water samples by extract weight (g) and percentage.

Sample	Neutrals		Asphaltenes		Acids		Bases		Amphoterics		Total
SHOP Project treater water (4 litre samples)											
Feb 1983	1.60	(75.6)	0.42	(19.8)	0.087	(4.1)	0.005	(0.2)	0.006	(0.3)	2.122
May 1983	2.07	(80.1)	0.44	(17.2)	0.052	(2.0)	0.017	(0.7)	--		2.583
Feb 1984	4.32	(84.5)	0.73	(14.2)	0.049	(0.9)	0.019	(0.4)	--		5.114
GREGOIRE LAKE Project (20 litre samples)											
GP-20 (Feb)	0.92[a]	(84.2)[b]	0.087[a]	(7.9)[b]	0.072[a]	(6.6)[b]	0.0072[a]	(0.66)[b]	0.0064[a]	(0.59)[b]	1.092
GP-20 (Mar)	1.05[c]	(99.3)					0.0068	(0.63)	0.0008	(0.07)	1.057
GP-21 (Feb)	0.68	(79.1)	0.12	(13.9)	0.048	(5.58)	0.0020	(0.23)	0.0072	(0.84)	0.86
GP-21 (Mar)	0.79[c]	(96.3)					0.0036	(0.44)	0.027	(3.29)	0.82
GP-21 (Jun)	15.8	(88.8)	1.47	(8.26)	0.47	(2.64)	0.038	(0.21)	0.0092	(0.05)	17.8
GP-26 (Feb)	0.23	(46.9)	0.0084	(1.71)	0.19	(38.8)	0.028	(5.71)	0.032	(6.65)	0.48
GP-26 (Mar)	3.98[c]	(98.3)					0.022	(0.54)	0.044	(1.09)	4.05
GP-26 (May)	4.41	(67.4)	1.68	(25.7)	0.33	(5.05)	0.051	(0.78)	0.073	(1.12)	6.54
GP-31 (Feb)	26.2	(69.9)	6.86	(18.3)	4.40	(11.7)	0.0068	(0.02)	0.016	(0.04)	37.5
GP-31 (Mar)	14.2	(100.0)					0.0084	(0.06)	0.014	(0.10)	14.2
GP-19 (May)	1.51	(65.1)	.37	(15.9)	.39	(16.8)	0.023	(0.99)	0.024	(1.03)	2.32
GP-19 (Jun)	3.07	(64.9)	1.09	(23.0)	.55	(11.6)	0.015	(0.32)	0.0090	(0.19)	4.73
UMATAC Wastewaters (4 litre samples, October 1982)											
Overhead	0.47	(13.5)	0.14	(4.0)	0.76	(21.9)	1.93	(55.8)	0.17	(5.0)	3.47
Preheat	0.37	(71.1)	0.023	(4.3)	0.05	(9.6)	0.05	(10.0)	0.026	(4.9)	0.52

[a] Numbers in this column indicate extract weight in grams.
[b] Numbers in this column indicate percentage of total extracted material.
[c] Contains asphaltenes and acids.

With one exception, the majority of the extracted material consisted of neutral compounds. The extractable material from the three SHOP samples was of similar composition with from 76 to 85% neutral compounds and 14 to 20% asphaltenes. The acids and bases represented a total of from 1.3 to 4.3% of the extractable material. The composition of the three samples taken over a one year period indicates that they were not produced from a zone which had undergone combustion.

The Gregoire Lake samples also contained mainly neutral material, 47 to 89%, and asphaltenes 2 to 25%. Large variations in the amount of neutral and asphaltene fractions are to be expected, as the samples consisted of material which was both dissolved and dispersed in the water. Some samples, notably GP-31, had large amounts of bituminous material associated with dispersed clay minerals. Samples of this type would be expected to have high asphaltene contents. In the Gregoire Lake samples acids represented from 2.6 to 39% of the extracted material. The high values indicate substantial alteration of the bitumen during in situ treatment. The amount of basic compounds also varied greatly, from 0.02 to 5.71%. Samples from the steam stimulated well GP-31 contained the smallest percentage of bases, whereas the COFCAW-produced fluids of GP-26 contained the highest percent bases. The amphoteric extract represented 0.07 to 6.6% of the extracted organic material. It is questionable whether these were true amphoteric compounds or material which was incompletely extracted under acidic or basic conditions. The GP-26 water collected in February is believed to have undergone rigorous thermal treatment and contained large amounts of iron. The total weight of extracted material ranged greatly from 0.49 to 37.5 g per sample. These values varied from those obtained by total organic carbon analysis. Such variations are not surprising considering the non-uniform nature of the oil-water-clay mineral mixtures which were sampled.

Wastewaters from the UMATAC process varied greatly in their organic carbon content (Table 4) and in the composition of the extractable organic material (Table 5). The overhead vent waters contained large amount of acids, 22% of the extractable material in the October 1982 sample, and large amounts of bases (56%). Neutral compounds comprised only 14%. In contrast the preheat vent waters contained 71% neutral compounds, 10% acids and 10% bases and had a much lower organic carbon content.

3.1.4 Detailed Chemical Analyses of SHOP Treated Waters.

3.1.4.1 Aromatic hydrocarbons. Studies of the carcinogenic properties of fossil fuels have historically focussed on the polycyclic aromatic hydrocarbon benzo(a)pyrene, but several other polycyclic aromatic hydrocarbons are known or suspected carcinogens. Benzo(a)pyrene was the first carcinogen to be isolated; it is a potent carcinogen, and it can be distinguished by its characteristic fluorescence spectrum. Benzo(a)pyrene can best be quantitatively measured in complex mixtures of organic compounds by gas chromotography-mass spectrometry on the basis of the single ion chromatogram of the molecular ion, mass 252 (Figure 2).

Low molecular weight aromatic compounds such as benzene and its alkylated homologues (masses 78, 92, 106, 120, 134, 148) and naphthalene and its homologues of mass 128, 142, 156, 170, and 184 are of interest because of their toxicity to aquatic organisms. Concentrations of water soluble hydrocarbons as low as 10 ppb produce sublethal effects in some organisms (in Harrison et al. 1975).

The aromatic hydrocarbons from the three SHOP project treater waters were analysed by GC/MS and the results are summarized in Table 6 and given in detail in Tables 6.1.1, 6.1.2 and 6.1.3 in Appendix 1. The most abundant compounds were the alkyl sustituted naphthalenes, especially compounds of mass 156, 170, and 184 with C2, C3, or C4 alkyl substitution. Second in abundance were the sulphur containing aromatic compounds, mainly alkyl substituted compounds of mass 212, 226, and 240. Third in order of abundance were the alkyl substituted phenanthrenes. Low molecular weight compounds are partly lost during the sample extraction and fractionation procedures so that the 1550 to 2296 ppb naphthalenes detected represent the minimum concentration of these compounds in the SHOP treater water samples.

Because of their volatility, naphthalene and alkylated naphthalenes were also measured as volatile components. Pure naphthalene

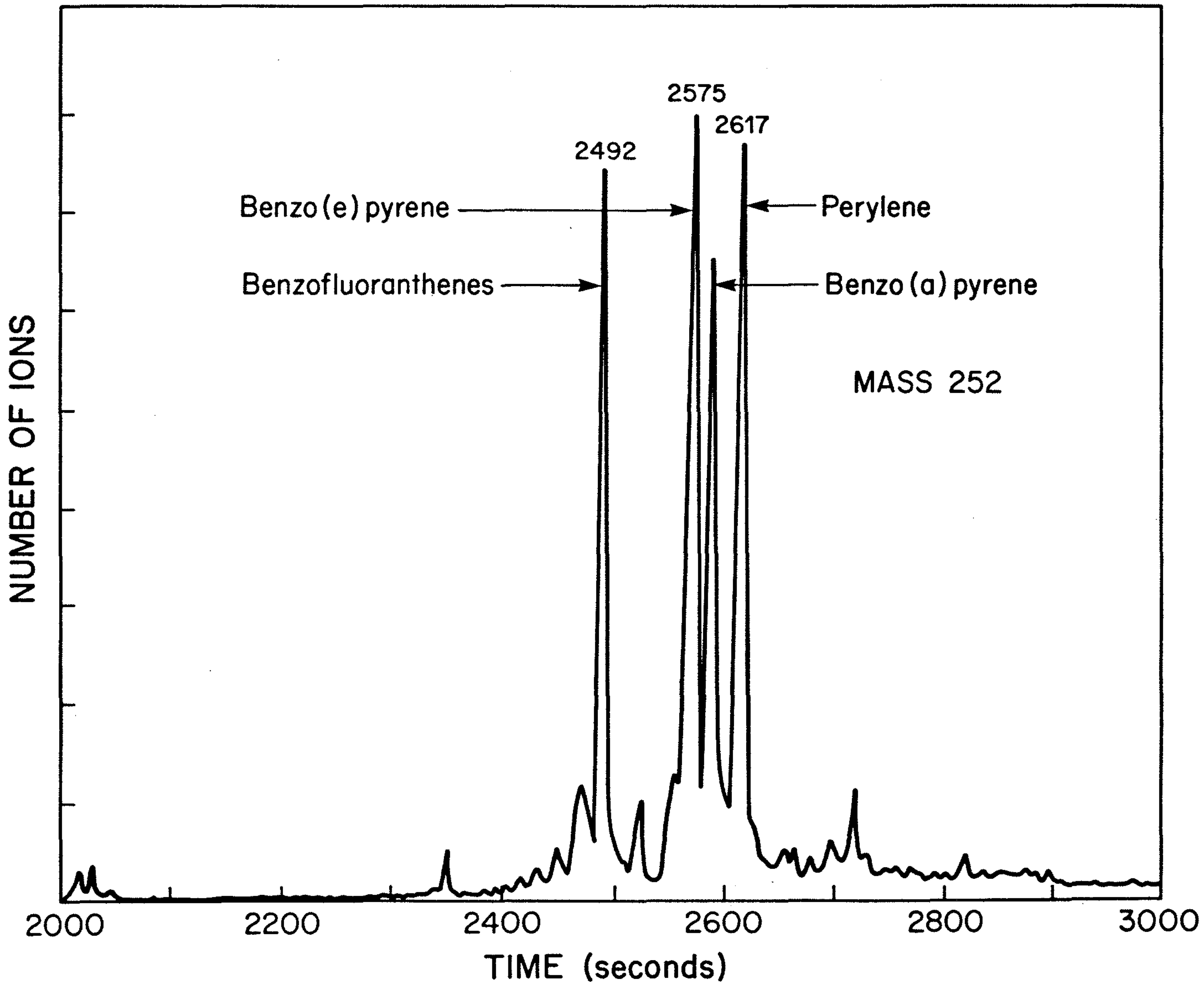

Figure 2. Single ion mass chromatogram (m.e. 252) of an aromatic fraction of GP26 oil.

Table 6. Extractable aromatic compounds in SHOP treater water samples (ppb).

Compound type Molecular weight	Sampling Date Jan 1983	 May 1983	 Feb 1984
napththalenes 128, 142, 156, 170, 184	1550	2296	1716
benzothiophenes 134, 148, 162, 176, 190, 204, 218	50	380	387
biphenyls 154, 168, 182	87	224	246
fluorenes 166, 180, 194, 208	175	308	227
phenanthrenes 178, 192, 206, 220	440	869	1488
dibenzothiophenes 184, 198, 212, 226, 240	595	1506	1937
fluoranthenes, pyrenes, benzofluorenes 202, 216, 230, 244, 258	86	17	90
chrysenes, triphenylenes, benz(a)anthracenes 228, 242, 256, 270	53	16	44
benzo(ghi)fluoranthenes 226, 240, 254, 268	ND	ND	ND
benzofluoranthenes 252	2	ND	ND
benzo(e)pyrene 252	4	ND	ND
benzo(a)pyrene 252	0.5	ND	ND
perylene 252	0.2	ND	ND
alkylated compounds 266, 280	11	ND	ND
benzo(ghi)perylene 276	0.5	ND	ND

ND - Not Determined

is soluble in water to the extent of 31.7 ppm, biphenyl to 7.0 ppm, and phenanthrene to 1.29 ppm (Mackay and Shiu 1977). The compounds are partitioned between the oil phase and the co-produced water phase in the SHOP samples; thus, their concentration in the water is more than one order of magnitude lower than for the pure compounds alone. In studies of oil-water systems by Anderson et al.(1974) a 10% South Louisiana crude oil-water solution at equilibrium had 300 ppb naphthalenes in solution and a bunker C residual oil gave 900 ppb. These values are in the range found for the January 1983 SHOP treater water.

Concentrations of the higher molecular weight compounds, mass 242 and higher, which are the most carcinogenic of the aromatic compounds, were low, in the case of benzo(a)pyrene the concentration was 0.5 ppm.

3.1.4.2 Other components. Acidic compounds were minor components of the SHOP treater waters as indicated by the dry weights in Table 5. Alkyl substituted benzoic acids and phenols were the main constituents identified, totalling 117 ppb in the January 1983 sample (Table 6.1.4, Appendix 1). The February 1984 sample also contained mainly alkyl substituted benzoic acids at 157 ppb, alkyl substituted phenols at 23 ppb, and alkyl substituted naphthenic acids at 20 ppb (Table 6.1.5, Appendix 1). Many of the more volatile acids and phenols would have been lost during sample preparation. Losses would have been greatest in samples taken to "dry weight" as in Table 5 but still would be substantial in samples prepared for GC/MS analysis, thus explaining the absence of phenol and methyl phenols.

Nitrogen containing compounds were present in very small quantities in the SHOP treater waters. Among the compounds identified in the SHOP treater water sample of February, 1984 were alkyl substituted; pyrazines, diaminobenzenes, quinolines, naphthylamines, and benzoquinolines (Table 6.1.6, Appendix 1). These compounds totalled only about 4 ppb.

3.1.5 Gregoire Lake Co-produced Waters

3.1.5.1 Aromatic and aliphatic hydrocarbons. Aromatic hydrocarbons were the most abundant group of organic compounds found in waters which had been co-produced with oil in the Gregoire Lake pilot study.

Samples of water from the Gregoire Lake pilot plant were collected in tightly capped vials and analysed for volatile organic compounds as described in 2.3.2. The compounds identified in each sample by the computerized library of the GC-MS are listed in the tables contained in Appendix 2. The approximate concentration of each component was calculated on the basis of the total organic carbon content of the sample and the relative abundance of each component based upon GC-MS. Regardless of the source of the sample (steam-produced or COFCAW-produced water) the volatile components were much the same: alkyl substituted benzenes, cyclohexanes and pentanes, and saturated normal or branched chain alkanes (Tables 6.2.1 to 6.2.12).

The May water sample from well GP26 (the COFCAW-produced water), contained 25 ppm toluene (methylbenzene), 29 ppm xylenes (dimethylbenzenes) and 13 ppm benzene (Table 6.2.8). (The concentrations in Appendix 2 were produced by computer and should be rounded off to two significant figures.) Aromatic compounds accounted for 65% of the volatile organic carbon or 18% of the total organic carbon. The steam-produced water, sampled in February from well GP31, also contained large amounts of low molecular weight aromatic compounds. Of the 242 ppm volatile organic carbon in this sample about 72 ppm were aromatic compounds and 24 ppm cyclopentanes and cyclohexanes (Table 6.2.9). The smaller proportion of aromatic hydrocarbons and the larger amount of cycloalkanes in the steam-produced water, as compared with the COFCAW-produced water, reflects the large amount of dispersed hydrocarbons in waters from well GP31. A second difference in samples GP26 (May) and GP31 (February) was the presence of about 3 ppm volatile sulphur compounds, thiophenes, in the COFCAW water. Aromatic sulphur compounds, benzothiophenes and dibenzothiophenes, were also found in the extractable neutral fraction of the COFCAW-produced waters from well GP26 (Table 6.2.13) but not in the steam-produced waters from GP19 (Table 6.2.14). These compounds were likely to have been in part generated by the combustion process. The composition of the hydrocarbons in the water reflects their physical state either as dispersed oil droplets or as dissolved hydrocarbons. The low molecular weight aromatic compounds such as alkyl substituted benzenes are preferentially dissolved from the oil into the water whereas the oil droplets consist mainly of aliphatic hydrocarbons. The cyclohexanes are among the more soluble of the aliphatic hydrocarbons, which accounts for their presence in the in-situ produced waters. The concentration of dissolved hydrocarbons in the produced waters depends upon a number of factors including the mole fraction of each hydrocarbon in the oil with which the water is in contact and the solubility of individual hydrocarbons. The concentration may be altered by partition with a gas phase and by loss by evaporation to the atmosphere. Since the solubility in water of benzene and alkyl substituted aromatic compounds is relatively high (1780 ppm for benzene) as compared with cycloalkanes (55 ppm for cyclohexane) and since the Henry's constants for aromatics are much lower than for alkanes, a predominance of aromatic compounds in the waters is to be expected.

The relationship between the chemical composition of water samples and their toxicity is discussed in Section 3.2.1.

3.1.5.2 Other compounds. The acidic components generally represented only a small proportion of the dissolved or dispersed organic compounds in the Gregoire Lake pilot waters (Table 5). Nevertheless, the concentrations, on the basis of possible biological effects, may be significant. The COFCAW produced water GP26, produced in May of 1981 and the corresponding steam-produced water from well GP19 contained 16 500 ppb and 19 500 ppb total acids, respectively, on the basis of the dried weight of extracted material. These two samples were analysed by GC/MS and the results are contained in Appendix 2, Tables 6.2.15 and 6.2.16. The major components in both samples were phenols and benzoic acids with phenols representing about 63% of the total acids. Phenol and methyl phenols in the GP26 water totalled 3140 ppb and C2- phenols totalled 2840 ppb (Table 6.2.15). The other major components were benzoic acid and its alkylated homologues. The concentration of benzoic acid was 1010 ppm and that of C1 to C3-benzoic acids was

470 ppb. The remaining components of the acidic fraction were aliphatic acids, naphthalene carboxylic acids, alcohols, and many oxygenated compounds in low concentrations. Losses of the more volatile components undoubtedly occurred during extraction and fractionation of the acidic compounds; therefore, the values reported are minimum concentration.

Interestingly, the steam-produced GP19 water contained similar types of compounds, but in slightly lower concentrations than the COFCAW-produced waters (Table 6.2.16). The high temperatures associated with the COFCAW process were expected to generate much higher concentrations of oxygenated compounds. The GP19, May treater water contained 113 ppb phenol, 1160 ppb methyl phenols, 2770 ppb C-2 phenols, 3510 ppb C-3 phenols, and 52 ppb C-4 phenols. The total phenols, 7600 ppb, represented about 45% of the acidic fraction as compared with 63% in the COFCAW water. Alkyl substituted benzoic acids accounted for a further 2260 ppb or 14% of the GP19 acids. The remaining compounds were naphthenic acids, alcohols and other oxygenated species.

The basic constituents of the Gregoire Lake Pilot GP26, May treater water were primarily quinolines and isoquinolines (Table 6.2.17). These components totalled 870 ppb, or 34% of the 2550 ppb total basic constituents. Other components identified were benzamines, cinnolines and benzoquinolines. Many compounds detected by GC/MS in the complex basic fraction could not be identified.

The steam-produced GP19 water (May) contained about 1150 ppb basic compounds (Table 6.2.18). Many compounds were not readily identifiable by GC/MS, but of those compounds which could be identified the major constituents were alkyl substituted benzamines, pyridines, quinolines, and indoles.

3.1.6 Combustion Tube Coproduced Waters

Insufficient sample size did not allow a rigorous analysis of waters co-produced with oil from the combustion tube experiments which were carried out by The University of Calgary, Chemical and Petroleum Engineering Department. Low molecular weight aromatic compounds were identified including biphenyls, phenanthrenes, and dibenzothiophenes.

Concentrations of these compounds were low, being 1 to 16 ppb (Table 6.3.1, Appendix 3). Numerous individual nitrogen compounds were found with concentrations up to 23 ppb (Table 6.3.2, Appendix 3). These included alkylated quinolines totalling 45 ppb, benzoquinolines totalling 80 ppb, and napthoquinolines totalling 10 ppb. These concentrations were low compared to waters produced by the COFCAW process.

3.1.7 UMATAC Process Wastewaters

Three types of wastewaters were obtained from the UMATAC process, overhead vent water, settling tank underflow and preheat vent water. Results of preliminary chemical analyses of samples obtained in October of 1982 are contained in Table 7. The overhead vent water and the preheat vent water showed high concentrations of dissolved organic carbon, 4910 ppm and 659 ppm, respectively. All samples had a low pH.

The overhead vent water contained many aromatic compounds, the most abundant of which are listed in Table 6.4.1 in Appendix 4. The majority of the compounds identified were naphthalenes, fluorenes, phenanthrenes, and dibenzothiophenes. Naphthalene and its C1-to-C4 alkylated homologues totalled 1960 ppb, fluorene and methyl fluorenes 97 ppb, phenanthrene and C1-to-C3 alkylated phenanthrenes 165 ppb, and dibenzothiophenes 99 ppb. Many of the lower molecular weight compounds such as benzene and methyl benzenes would have been lost during sample preparation as would some of the naphthalenes. These concentrations of low molecular weight aromatic compounds are of biological concern as will be discussed in Section 3.2. Also found was the carcinogen benzo(a)pyrene at a concentration of 5 ppb.

The preheat vent water contained many aromatic componds but in lower concentrations than the overhead vent waters (Table 6.4.2, Appendix 2). As with the overhead waters, the major constituents of the preheat vent waters were alkylated naphthalenes, fluorenes, dibenzothiophenes, and phenanthrenes. Benzo(a)pyrene was found in low concentrations of approximately 0.2 ppb.

The most abundant compounds identified in the overhead vent waters were found in the basic fraction of the sample. Many alkyl substituted pyridines, pyrimidines, quinolines, aminodans, and aminobiphenyls were detected (Table 6.4.3, Appendix 4). The lower molecular

Table 7. Carbon content and acidity of UMATAC water samples.

1.	Overhead vent water, pH 4.4	
	Total carbon content	5070 ppm
	Total organic carbon content	4910 ppm
	Volatile carbon content	424 ppm
	Phenols, substituted phenols, and related compounds	240 ppm
	Bases, primarily nitrogen containing compounds	480 ppm
	Neutral compounds, primarily aromatic hydrocarbons	120 ppm
	Amphoteric compounds	45 ppm
2.	Settling tank underflow water, pH 2.8	
	Total carbon content	71 ppm
	Total organic carbon content	69 ppm
	Volatile carbon content	1 ppm
	Phenols and related compounds	1 ppm
	Bases	1 ppm
	Neutral compounds	1 ppm
3.	Preheat vent water, pH 2.5	
	Total carbon content	703 ppm
	Total organic carbon content	659 ppm
	Volatile carbon content	22 ppm
	Phenols, substituted phenols, and related compounds	19 ppm
	Bases, nitrogen containing compounds	13 ppm
	Neutral compounds, aromatic hydrocarbons	160 ppm
	Amphoteric compounds	6 ppm

weight compounds were the most abundant with 29 000 ppb of a single methyl pyrimidine and 20 000 ppb of a dimethyl pyrimidine. Alkyl pyridines totalled 52 000 ppb, alkyl pyrimidines totalled 29 200 ppb, and alkyl quinolines totalled 15 700 ppb. Quinoline and some methylquinoline isomers are mutagenic and carcinogenic. Similarly, some aminobiphenyl and diaminobiphenyl isomers are also carcinogenic or mutagenic. These groups of compounds were present at concentrations totalling 1000 ppb.

3.2 CHEMICAL ANALYSIS OF PRODUCED OILS, RELATED PRODUCTS, AND RESIDUALS

Aromatic compounds containing three or more aromatic rings were separated from produced oils from the SHOP project, the Gregoire Lake pilot, the UMATAC pilot plant, the Peace River pilot project, and combustion tube experiments. In addition, Athabasca bitumen, fractions of the Peace River oil, and diesel fuel used in the Gregoire Lake pilot were analysed. To put the above samples into perspective the composition of refinery residuals and tars was also investigated.

The aromatic hydrocarbons were extracted from the oils with dimethylformamide. This crude aromatic extract was further purified by column chromatography and the separated aromatic hydrocarbons analysed by GC/MS.

3.2.1 SHOP Wellhead Oils

Summarized results for the SHOP wellhead oils are contained in Table 8 with more complete data in Appendix 5, Tables 6.5.1 to 6.5.5. The major aromatic components of the SHOP oils were alkylated phenanthrenes which ranged in concentration from 793 ppm in the oil from well P2 collected in January to 2379 ppm in the well P1 January sample. Other major constituents were the alkylated fluorenes and alkylated pyrenes and benzofluorenes in the mass range 202 to 286. Fluorene and alkylated fluorenes totalled from 251 to 639 ppm whereas the fluoranthene-pyrene-benzo(a)anthracene groups totalled from 123 to 514 ppm. Lesser amounts of the known mutagenic and carcinogenic compounds benzo(a)pyrene, benzo(e)pyrene, and perylene were found. The amounts of benzo(a)pyrene in the SHOP and other oils are shown in Table 9. Benzo(a)pyrene in the

Table 8. Polycyclic aromatic hydrocarbons in heavy oils from the SHOP project (ug/g of original oil).

	Sample Description and Number						
	1983 February					1983 May	
Compound Type, Molecular Ions	Base Oil	P1	P2	P3	P4	P1	P3
fluorenes 166, 180, 194, 208, 222	639	360	265	447	496	251	434
phenanthrenes, anthracenes 178, 192, 206, 220, 234	2152	2379	793	1051	1302	1184	1738
fluoranthenes, pyrenes, benzofluorenes 202, 216, 230, 244, 258, 272, 286	380	514	282	211	123	295	419
chrysenes, triphenylenes, benz(a)anthracenes 228, 242, 256, 270, 284, 298	189	372	182	135	55	148	221
benzo(ghi)fluoranthenes 226, 240, 254, 268	ND	ND	ND	ND	ND	ND	--
benzofluoranthenes 252	4.6	7.0	3.8	4.1	0.95	3.0	6.0
benzo(e)pyrenes 252	18	17	8.9	8.8	2.49	8.0	14
benzo(a)pyrene 252	7.5	1.9	1.7	1.6	ND	1.5	3.0
perylene 252	3.9	ND	ND	ND	ND	ND	ND
alkylated compounds 266, 280, 294	18	16	20	14	4.3	14.5	23
276, 290, 304	ND	1	2	ND	ND	1	3.0

ND = Not determined

SHOP oil samples ranged in concentration from 1.5 to 7.5 ppm. This is in the range for most light to medium weight crude oils and no evidence was found in these samples of the generation of carcinogenic hydrocarbons by the SHOP in situ combustion process. It should, however, be noted that these samples likely do not represent oils from the combustion zone.

3.2.2 Gregoire Lake and Related Oils

Oils produced from the Gregoire Lake pilot, Athabasca bitumen, and commercial synthetic crude oil from the Fort McMurray area were also analysed for benzo(a)pyrene. These included: (1) oil from well GP26 produced by the COFCAW process; (2) oil from well GP19 produced by steam stimulation; (3) bitumen produced by a hot water extraction process; (4) Suncor synthetic crude oil; and (5) diesel fuel circulated downhole to prevent blockages.

The benzo(a)pyrene content of the COFCAW-produced oil sampled in 1981 ranged up to 14 µg/g of oil (Table 9). The produced oil was a mixture of diesel fuel and bitumen together with combustion products; thus, the combustion products themselves likely contained much higher concentratios of benzo(a)pyrene. Tubing samples contained low concentrations of benzo(a)pyrene, the range being 2.1 to 4.2 µg/g. Steam-produced oil from well GP19 contained 4.5 µg of benzo(a)pyrene per gram of oil, and bitumen contained 1.5 µg/g. No benzo(a)pyrene was detected in the diesel fuel but synthetic crude oil contained 3.9 µg/g. The method developed for measuring the benzo(a)pyrene content of heavy oils in this project gave reproducible results. Triplicate analysis of a sample of GP26 oil gave values of 7.5, 8.1, and 8.8 µg/g.

It has been postulated that the COFCAW process would generate polynuclear aromatic hydrocarbons from the cyclic components of the Athabasca bitumen. This was apparently true, with the benzo(a)pyrene content of the COFCAW-produced oil being at least ten times greater than that of the hot water-produced bitumen. The steam-produced oil contained three times as much benzo(a)pyrene as the bitumen. It is not known whether this was the result of thermal action from the injected stream or if there was communication to areas which had undergone fire-flood tests. Interestingly, the steam-produced oil contained about the

Table 9. The benzo(a)pyrene content of heavy oils and related products.

Sample	B(a)P Content (ug/g)
SOUTHERN ALBERTA PROJECT	
Treater oil, 1983 January	2.1
Well No. 1, 1983 February	1.9
Well No. 2, 1983 February	1.7
Well No. 3, 1983 February	1.6
Well No. 1, 1983 May	1.5
Well No. 3, 1983 May	3.0
Base Oil	7.5
UMATAC PROCESS	
Day tank	16
Overhead oil	2.9
COMBUSTION TUBE EXPERIMENT	
159-11 heavy oil	2.6
159-14 heavy oil	4.2
PEACE RIVER PROJECT	
Steam-produced emulsion	2.7
Vacuum gas oil	1.7
Top oil	0.1
Pitch	1.9
REFINERY PRODUCTS	
Steam cracker tar	154
Catalytic cracker heavy oil	240
Fluid coker heavy gas oil	91
Catalytic cracker fractionator bottoms	1050
GREGOIRE LAKE IN-SITU PROJECT	
Heavy oil	7.5-14
Bitumen	1.5
Steam-produced oil	4.5
Tubing samples	2.1-4.2
Diesel fuel	0.1
OTHER OILS	
Most crude oils	3-1
Some asphaltic oils	1-20
Athabasca synthetic crude oil	3.9
Coal liquefaction products	2-180
Shale oil	3

same amount of benzo(a)pyrene as the hydrotreated synthetic crude oil produced by Suncor.

Comparisons with published values for the benzo(a)pyrene content of other oils and fuels must be viewed with some reservations. Until the advent of high resolution capillary gas chromatographic columns with coupled mass spectrometry and deuterated internal standards, the quantitative analysis of benzo(a)pyrene in complex hydrocarbon mixtures was difficult. Conventional crude oils generally contain 1 to 3 µg/g benzo(a)pyrene with some asphaltic oils containing up to 20 µg/g and coal liquefaction products containing up to 180 µg/g (Table 10).

If benzo(a)pyrene alone were considered as an indicator of the carcinogenic potential of the COFCAW-produced oil, it is clear that any health hazard would, on the basis of present data, be no greater than that of some asphaltic oils.

Although benzo(a)pyrene is the only carcinogen which has been widely measured in fossil fuels, several other aromatic hydrocarbons are known or suspected to be carcinogenic. Further, the potency of some carcinogens is enhanced by the presence of paraffinic and other aromatic hydrocarbons. For example, benzo(a)pyrene applied to mouse skin as a solution in n-dodecane is 1000 times more potent than a similar benzene solution.

Other carcinogens and mutagens are listed in Tables 11 to 13. Among them are the aromatic compounds: alkylsubstituted phenanthrenes and anthracenes of masses 192, 206, and 220; benz(a)anthracene and benzo(c)phenanthrene of mass 228; methylsubstituted chrysenes, benz(a)-fluoranthene of mass 252; benzo(c)chrysene, benzo(g)chrysene and several dibenzanthracenes of mass 278; benzo(ghi)perylene and o-pheny-lene-pyrene of mass 276; and several dibenzopyrene isomers of mass 302. Numerous compounds with the appropriate masses were found in the COFCAW and steam-produced oils and in synthetic crude oil. These compounds far exceeded benzo(a)pyrene in abundance. For example, the COFCAW oil contained 26 µg/g benz(a)anthracene and 140 µg/g of other aromatic hydrocarbons of mass 228. Compounds of mass 242 totalled 190 µg/g and of mass 256 totalled 145 µg/g. Compounds of mass 252, other than benzo(a)-pyrene, totalled 43 µg/g. Compounds of mass greater than 252 were far less abundant with mass 276 and 278 compounds accounting for only 1 µg/g

Table 10. Benzo(a)pyrene content of petroleum and related materials.

Material	Concentration (ppm)	Source
Crude Oil		
Libia	1.3	M.R. Guerin 1977
Venezuala	1.6	M.R. Guerin 1977
Persian Gulf	0.04	M.R. Guerin 1977
Arabian	1.5	M.R. Guerin 1977
Kuwait	2.8	Coomes and Hazer 1982
South Louisiana	1.2	Coomes and Hazer 1982
Petroleum	3	Tomkins et al. 1981
Wilmington	1	Tomkins et al. 1981
Texas	20	Bingham and Barkley 1979
Asphaltic	5	Bingham and Barkley 1979
Paraho	13.6	Holland and Stafford 1981
Paraho-hydrotreated	17.7	Holland and Stafford 1981
Shale derived	3.1	M.R. Guerin 1977
Shale derived-hydrotreated	0.7	M.R. Guerin 1977
Coal derived	3	M.R. Guerin 1977
Shale Oil		
Raw	0.015	M.R. Guerin 1977
Processed	0.03	M.R. Guerin 1977
Tosco raw	3.7	Coomes and Hazer 1982
Tosco hydrotreated (0.25%N)	0.7	Coomes and Hazer 1982
AP-79-4 raw	2.0	Coomes and Hazer 1982
AP-79-3 hydrotreated (0.33%N)	10.0	Coomes and Hazer 1982
Colorado raw	3.2	R.M. Coomes 1979
Certified	32	Tomkins et al. 1981

continued...

Table 10. Continued.

Material	Concentration (ppm)	Source
Petroleum Products		
Gasoline	0.4	M.R. Guerin 1977
Heating oil, No. 2	0.03	M.R. Guerin 1977
Industrial fuel oil	1000	Bingham and Barkley 1979
Lubricating oil, new	0	Durand and Petroff 1980
Lubricating oil, used	5	Durand and Petroff 1980
Diesel fuel	0.05	M.R. Guerin 1977
Recycled Oils		
Motor oil, new	0.03	M.R. Guerin 1977
Motor oil, used	4.0	M.R. Guerin 1977
Virgin Motor Oil A	0.12	Brown et al. 1980
Virgin Motor Oil B	0.07	Brown et al. 1980
Virgin Motor Oil C	0.06	Brown et al. 1980
Used motor oil (composite)	11	Brown et al. 1980
Used railroad diesel oil	10	Brown et al. 1980
Used motor oil (unleaded, 4,145 Miles)	14	Brown et al. 1980
Used synthetic motor oil (23,000 miles)	16	Brown et al. 1980
Used gasoline automotive crank case oil	15	Brown et al. 1980
Used gasoline automotive crank case oil	13	Brown et al. 1980
Re-refiner's feedstock waste oil (Sampling Period A)	13	Brown et al. 1980

continued...

Table 10. Continued.

Material	Concentration (ppm)	Source
Re-refiner's feedstock waste oil (Sampling Period B)	8.8	Brown et al. 1980
Service station waste oil (Station A)	5.3	Brown et al. 1980
Service station waste oil (Station B)	3.2	Brown et al. 1980
No. 4 Virgin residual fuel oil (Source A)	2.1	Brown et al. 1980
No. 5 Virgin residual fuel oil (Source B)	2.8	Brown et al. 1980
No. 5 Virgin residual fuel oil (duplicate of Source B)	3.3	Brown et al. 1980
No. 6 Virgin residual fuel oil (Bunker C, Source A)	26.5	Brown et al. 1980
No. 6 Virgin residual fuel oil (Bunker C, Source B)	35	Brown et al. 1980
Recycled distillate fuel oil	7.7	Brown et al. 1980
No. 5 recycled fuel oil (Company A)	8.4	Brown et al. 1980
No. 5 recycled fuel oil (Company B)	10.5	Brown et al. 1980
Reprocessed oil (Company C)	10.5	Brown et al. 1980
Re-refined motor oil	2.1	Brown et al. 1980
Recycled liquid pyrolysis product from tires	161	Brown et al. 1980

continued...

Table 10. Concluded.

Material	Concentration (ppm)	Source
Miscellaneous		
Coal	4	R.M. Coomes 1979
Coal oil	150	Tomkins et al. 1981
Coal liquid oil (SRC-11)	180	Tomkins et al. 1981
Coal tar	3000	M.R. Guerin 1977
Coal tar pitch	10000	M.R. Guerin 1977
Petroleum pitch	2000	M.R. Guerin 1977
Bitumen coal	0.001	M.R. Guerin 1977
Creasote	200	M.R. Guerin 1977
Asphalt	2.0	M.R. Guerin 1977
Asphalt	10-100	R.M. Coomes 1979
Residium (catalytically cracked)	4000	Bingham and Barkley 1979
Paraffinic distillate	1	Bingham and Barkley 1979

Table 11. Mutagenic and carcinogenic aromatic hydrocarbons.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
1-ring			
Benzene	–	+	DeFlora et al. 1984
2-ring			
Naphthalene	–	–	McCann et al. 1975
1-Methylnaphthalene	(+,-)		Kimball and Munro 1981
			Kaden et al. 1979
2,6-Dimethylnaphthalene	–		Kaden et al. 1979
3-ring			
Acenaphthene	+		Epler et al. 1979
Acenaphthylene	+		Kaden et al. 1979
Anthracene	–	–	La Voie et al. 1983
			DeFlora et al. 1984
1-Methylanthracene	–	–	La Voie et al. 1983
			Kimball and Munro 1981
2-Methylanthracene	(+,-)		La Voie et al. 1979
			Kimball and Munro 1981
9-Methylanthracene	+	–	Dipple 1976
			Kaden et al. 1979
9,10-Dimethylanthracene	+	+	Kimball and Munro 1981
			La Voie et al. 1983
Fluorene	–	–	La Voie et al. 1979
			Kimball and Munro 1981
1-Methylfluorene	–		La Voie et al. 1979
2-Methylfluorene	–		La Voie et al. 1979
3-Methylfluorene	–		La Voie et al. 1979
4-Methylfluorene	–		La Voie et al. 1979
9-Methylfluorene	+	–	La Voie et al. 1981
			La Voie et al. 1979

continued...

Table 11. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
1,9-Dimethylfluorene	+	-	La Voie et al. 1983
			La Voie et al. 1979
2,3-Dimethylfluorene	-		La Voie et al. 1979
9,9-Dimethylfluorene	-		La Voie et al. 1979
9-Ethylfluorene	+		La Voie et al. 1979
9-n-Propylfluorene	+		La Voie et al. 1979
9-i-Propylfluorene	-		La Voie et al. 1979
9-Phenylfluorene	-		La Voie et al. 1979
Phenanthrene	(+,-)	-	Kimball and Munro 1981
			Nat. Acad. Sci. 1972
			La Voie et al. 1979
1-Methylphenanthrene	+	+	La Voie et al. 1983
			Dipple 1976
2-Methylphenanthrene	(+,-)		Kaden et al. 1979
			La Voie et al. 1979
3-Methylphenanthrene	-		La Voie et al. 1983
4-Methylphenanthrene	-		La Voie et al. 1983
9-Methylphenanthrene	+		La Voie et al. 1983
1,4-Dimethylphenanthrene	+	+	La Voie et al. 1983
			Dipple 1976
1,9-Dimethylphenanthrene	-	-	La Voie et al. 1983
			Dipple 1976
2,7-Dimethylphenanthrene	-		La Voie et al. 1983
3,6-Dimethylphenanthrene	-		La Voie et al. 1983
4,5-Dimethylphenanthrene	-		La Voie et al. 1983
4,9-Dimethylphenanthrene	-		La Voie et al. 1983
4,10-Dimethylphenanthrene	+		La Voie et al. 1983
1,2,4-Trimethylphenanthrene		+	Dipple 1976

continued...

Table 11. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
1,2,3,4-Tetramethylphenanthrene		+	Dipple 1976
2,4,5,7-Tetramethylphenanthrene	–		La Voie et al. 1983
3,4,5,6-Tetramethylphenanthrene	–		La Voie et al. 1983
2-Ethylphenanthrene	–		La Voie et al. 1983
3-Ethylphenanthrene	–		La Voie et al. 1983
9-Ethylphenanthrene	–		La Voie et al. 1983
9-Propylphenanthrene	–		La Voie et al. 1983
9-Isopropylphenanthrene	–		La Voie et al. 1983
9-Florophenanthrene	+		La Voie et al. 1983
9-Chlorophenanthrene	+		La Voie et al. 1983
9-Bromophenanthrene	+		La Voie et al. 1983
<u>4-ring</u>			
Benz(a)anthracene	+	+	DeFlora et al. 1984
1-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
2-Methylbenz(a)anthracene	+	(+,-)	Coombs et al. 1976 Dipple 1976
3-Methylbenz(a)anthracene	+	(+,-)	Coombs et al. 1976 Dipple 1976
4-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
5-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
6-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
7-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
8-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
9-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
10-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
11-Methylbenz(a)anthracene	+	+	Coombs et al. 1976
12-Methylbenz(a)anthracene	+	+	Coombs et al. 1976

continued...

Table 11. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
1,12-Dimethylbenz(a)anthracene		-	Dipple 1976
4,5-Dimethylbenz(a)anthracene		+	Dipple 1976
6,7-Dimethylbenz(a)anthracene		+	Dipple 1976
6,8-Dimethylbenz(a)anthracene		+	Dipple 1976
6,12-Dimethylbenz(a)anthracene		+	Dipple 1976
7,8-Dimethylbenz(a)anthracene		+	Dipple 1976
7,11-Dimethylbenz(a)anthracene		+	Dipple 1976
7,12-Dimethylbenz(a)anthracene	+	+	Nat. Acad. Sci. 1972 Coombs et al. 1976
8,9-Dimethylbenz(a)anthracene		+	Dipple 1976
8,12-Dimethylbenz(a)anthracene		+	Dipple 1976
9,10-Dimethylbenz(a)anthracene	+	+	Kimball and Munro 1981 Rinkus and Legator 1979
9,11-Dimethylbenz(a)anthracene		+	Dipple 1976
4,5,10-Trimethylbenz(a)anthracene		+	Dipple 1976
4,7,12-Trimethylbenz(a)anthracene		+	Dipple 1976
6,7,8-Trimethylbenz(a)anthracene		+	Dipple 1976
6,7,12-Trimethylbenz(a)anthracene		+	Dipple 1976
6,8,12-Trimethylbenz(a)anthracene		+	Dipple 1976
7,8,12-Trimethylbenz(a)anthracene		+	Dipple 1976
7,9,12-Trimethylbenz(a)anthracene		+	Dipple 1976
7,8,9,12-Tetramethylbenz(a)-anthracene	+		Dipple 1976
7,9,10,12-Tetramethylbenz(a)-anthracene	+		Dipple 1976
Benzo(a)fluorene	-	-	Nat. Acad. Sci. 1972 La Voie et al. 1979
Benzo(b)fluorene	(+,-)	-	Nat. Acad. Sci. 1972 La Voie et al. 1979 Kimball and Munro 1981

continued...

Table 11. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
Benzo(c)fluorene	–	–	Nat. Acad. Sci. 1972
			La Voie et al. 1979
11-Methylbenzo(a)fluorene	+	–	La Voie et al. 1979
			La Voie et al. 1981
11-Methylbenzo(a)fluorene	+	+	La Voie et al. 1979
			La Voie et al. 1981
7-Methylbenzo(c)fluorene	+	–	La Voie et al. 1979
			La Voie et al. 1981
Benzo(c)phenanthrene		+	Nat. Acad. Sci. 1972
2-Methylbenzo(c)phenanthrene		+	Dipple 1976
3-Methylbenzo(c)phenanthrene		+	Dipple 1976
4-Methylbenzo(c)phenanthrene		+	Dipple 1976
5-Methylbenzo(c)phenanthrene		+	Dipple 1976
6-Methylbenzo(c)phenanthrene		+	Dipple 1976
5-Ethylbenzo(c)phenanthrene		+	Dipple 1976
Chrysene	+	+	Nat. Acad. Sci. 1972
			Coombs et al. 1976
1-Methylchrysene	+		Coombs et al. 1976
2-Methylchrysene	+	+	Kimball and Munro 1981
			Coombs et al. 1976
3-Methylchrysene	+	+	Kimball and Munro 1981
			Coombs et al. 1976
4-Methylchrysene	+	+	Kimball and Munro
			Coombs et al. 1976
5-Methylchrysene	+	+	Kimball and Munro 1981
			Coombs et al. 1976
6-Methylchrysene	+	+	Kimball and Munro 1981
			Coombs et al. 1976

continued...

Table 11. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
4,5-Dimethylchrysene		+	La Voie et al. 1983
5,6-Dimethylchrysene		+	Dipple 1976
1,11-Dimethylchrysene	+	+	Coombs et al. 1976
Fluoranthene	+	-	Nat. Acad. Sci. 1972 Kimball and Munro 1981
Pyrene	(+,-)	-	McCann et al. 1975 Kimball and Munro 1981
1-Methylpyrene	+	+	Kaden et al. 1979
Triphenylene	+	-	Kaden et al. 1979
1-Methyltriphenylene		-	Dipple 1976
1,4-Dimethyltriphenylene		-	Dipple 1976
<u>5-ring</u>			
Benzo(c)chrysene		+	Dipple 1976
Benzo(g)chrysene		+	Dipple 1976
Benzo(a)pyrene	+	+	Kaden et al. 1979
2-Methylbenzo(a)pyrene		+	Dipple 1976
3-Methylbenzo(a)pyrene		+	Dipple 1976
4-Methylbenzo(a)pyrene		+	Dipple 1976
5-Methylbenzo(a)pyrene		+	Dipple 1976
6-Methylbenzo(a)pyrene		+	Dipple 1976
7-Methylbenzo(a)pyrene		+	Dipple 1976
11-Methylbenzo(a)pyrene		+	Dipple 1976
12-Methylbenzo(a)pyrene		+	Dipple 1976
4,5-Dimethylbenzo(a)pyrene		+	Dipple 1976
3,12-Dimethylbenzo(a)pyrene		+	Dipple 1976
3,6-Dimethylbenzo(a)pyrene		+	Dipple 1976
2,3-Dimethylbenzo(a)pyrene		+	Dipple 1976
1,6-Dimethylbenzo(a)pyrene		+	Dipple 1976

continued...

Table 11. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
1,4-Dimethylbenzo(a)pyrene		+	Dipple 1976
1,3-Dimethylbenzo(a)pyrene		+	Dipple 1976
1,2-Dimethylbenzo(a)pyrene		+	Dipple 1976
1,3,6-Trimethylbenzo(a)pyrene		+	Dipple 1976
Benzo(e)pyrene	+	(+,-)	Nat. Acad. Sci. 1972 Kaden et al. 1979
Benzo(b)fluoranthene	+	+	Nat. Acad. Sci. 1972 Kaden et al. 1979
Benzo(j)fluoranthene	+	+	Nat. Acad. Sci. 1972 Kaden et al. 1979
Benzo(k)fluoranthene	+	-	Nat. Acad. Sci. 1972 Kaden et al. 1979
Benzo(g,h,i)fluoranthene		-	Nat. Acad. Sci. 1972
Dibenz(a,c)anthracene	+	+	McCann et al. 1975
Dibenz(a,j)anthracene		+	Nat. Acad. Sci. 1972
Dibenz(a,h)anthracene	+	+	McCann et al. 1975
Dibenz(de,kl)anthracene	+	-	DeFlora et al. 1984
2-Methyldibenz(a,h)anthracene		+	Dipple 1976
2-Methyldibenz(a,h)anthracene		+	Dipple 1976
6-Methyldibenz(a,h)anthracene		+	Dipple 1976
Dibenzo(a,g)fluorene		+	Nat. Acad. Sci. 1972
Dibenzo(a,c)fluorene		+	Nat. Acad. Sci. 1972
Dibenzo(a,h)fluorene		+	Nat. Acad. Sci. 1972
10-Methyldibenz(a,c)fluorene		+	Dipple 1976
Cholanthrene		+	Nat. Acad. Sci. 1972
3-Methylchlanthracene	+	+	McCann et al. 1975
Dibenzo(c,g)phenanthrene		-	Dipple 1976
Dibenzo(b,g)phenanthrene		-	Dipple 1976
Perylene	+	-	Kaden et al. 1979

continued...

Table 11. Concluded.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
<u>6-ring</u>			
Benzo(r,s,t)pentaphene	+	+	Helmes et al. 1982
Benzo(g,h,i)peryelene	+	+	Kaden et al. 1979
Dibenzo(b,def)chrysene		+	Dipple 1976
Dibenzo(def,p)chrysene		+	Dipple 1976
Dibenzo(a,l)pyrene		+	Nat. Acad. Sci. 1972
Dibenzo(a,h)pyrene		+	Nat. Acad. Sci. 1972
Dibenzo(a,i)pyrene	+	+	McCann et al. 1975
Dibenzo(cd,jk)pyrene	+	(+,-)	Dipple 1976 Kaden et al. 1979
Dibenz(b,e)fluoranthene	+		Kaden et al. 1979

+ = mutagenic or carcinogenic activity

- = no mutagenic or carcinogenic activity detected

Table 12. Mutagenic and carcinogenic nitrogen compounds.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
Dimethylamine	+		Helmes et al. 1982
<u>1-ring</u>			
1-Nitroaniline	-		DeFlora et al. 1984
Aniline	-	-	McCann et al. 1975 Epler et al. 1979
2-Methylaniline	-		Kimball and Munro 1981
3-Methylaniline	-		Kimball and Munro 1981
4-Methylaniline	-		Kimball and Munro 1981
2,3-Dimethylaniline	-		Kimball and Munro 1981
2,4-Dimethylaniline	-		Kimball and Munro 1981
2,5-Dimethylaniline	+		Kimball and Munro 1981
2,6-Dimethylaniline	-		Kimball and Munro 1981
3,4-Dimethylaniline	-		Kimball and Munro 1981
2,4,6-Trimethylaniline	(+,-)		Kimball and Munro 1981, Epler et al. 1979
Auramine	-	+	McCann et al. 1975
Pyridine	(+,-)	-	Kimball and Munro 1981 Kaden et al. 1979
Pyrrole	-		Kimball and Munro 1981
4-Aminophenol	-	-	DeFlora et al. 1984
2-Aminophenol	(+,-)	-	DeFlora et al. 1984 Kimball and Munro 1981
3-Methyl-4-dimethyl-aminoazobenzene	+		McCann et al. 1975
N-Methyl-4-aminobenzene	+	+	McCann et al. 1975
Phenylhydroxylamine	-		Nohmi et al. 1984
2,4-Diaminotoluene	+	+	Rinkus and Legator 1979

continued...

Table 12. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
<u>2-ring</u>			
1-Nitronaphthalene	-		Klopman and Rosenkranz 1984
2-Nitronaphthalene	(+,-)	+	DeFlora et al. 1984
			Klopman and Rosenkranz 1984
1,3-Dinitronaphthalene	-		Klopman and Rosenkranz 1984
1,5-Dinitronaphthalene	-		Klopman and Rosenkranz 1984
Biphenyl	-	+	Kimball and Munro 1981
			Rinkus and Legator 1979
2-Aminobiphenyl	+		McCann et al. 1975
			Kimball and Munro 1981
4-Aminobiphenyl	+	+	Kimball and Munro 1981
4-Chlorobiphenyl	-		Schoeny 1982
4-Chloromethylbiphenyl	+		Ladner 1982
4-Hydroxymethylbiphenyl	-		Ladner 1982
2,3'-Dimethyl-4-Aminobiphenyl	+	+	McCann et al. 1975
4-4-Diaminobiphenyl(benzidine)	+	+	McCann et al. 1975
3,3'-Dimethylbenzidine		+	Rinkus and Legator 1979
3,3',5,5'-Tetramethylbenzidine	-	-	McCann et al. 1975
N,N,N',N'-Tetramethllbenzidine	-	-	McCann et al. 1975
1-Naphthylamine	+	-	McCann et al. 1975
2-Naphthylamine	+	+	McCann et al. 1975
1-Aminonaphthalene	+	+	Kimball and Munro 1981
2-Aminonaphthalene	+	+	Kimball and Munro 1981
3-Methyl-2-Naphthylamine		+	Rinkus and Legator 1979
Quinoline	+		Kimball and Munro 1981
1-Methylquinoline	+		Kimball and Munro 1981
2-Methylquinoline	-		Kaden et al. 1979
4-Methylquinoline	+		Kaden et al. 1979
7-Methylquinoline	+		Epler et al. 1979
8-Methylquinoline	+		Epler et al. 1979

continued...

Table 12. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
2,6-Dimethylquinoline	-		Epler et al. 1979
2,7-Dimethylquinoline	-		Kaden et al. 1979
8-Aminoquinoline	+		Epler et al. 1979
Isoquinoline	-		Seixas et al. 1982
1-Methylisoquinoline	-		Kaden et al. 1979
3-Methylisoquinoline	-		Kaden et al. 1979
Indole	-	-	Kaden et al. 1979
2-Methylindole	-		Kimball and Munro 1981
3-Methylindole	-		Kimball and Munro 1981
2-Phenylpyridine	-		Kaden et al. 1979
4-Phenylpyridine	+		Kaden et al. 1979
Naphthoquinone	-		Tikkanen et al. 1983
<u>3-ring</u>			
5-Nitroacenaphthene	+	+	Rinkus and Legator 1979
9-Nitroanthracene	-	-	Pitts, Jr. et al. 1982 Klopman and Rosenkranz 1984
2-Nitrofluorene	+	+	McCann et al. 1975
2,7-Dinitrofluorene	+	+	Klopman and Rosenkranz 1984
2-Nitrophenanthrene	-		Klopman and Rosenkranz 1984
3,4-Benzoquinoline	+		Kaden et al. 1979
5,6-Benzoquinoline	+	+	Kaden et al. 1979
7,8-Benzoquinoline	+		Kaden et al. 1979
Dibenzofuran	-		Schoeny 1982
1-Aminophenanthrene	+		Later et al. 1983
2-Aminophenanthrene	+		Later et al. 1983
3-Aminophenanthrene	+		Later et al. 1983
4-Aminophenanthrene	-		Later et al. 1983
9-Aminophenanthrene	+		Later et al. 1983
1H-Benz(g)indole	-		Kaden et al. 1979

continued...

Table 12. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
Acridine	+	–	Seixas et al. 1982 Nat. Acad. Sci. 1972
9-Aminoacridine	+	+	Lee and Castle 1981 McCann et al. 1975
Carbazole	–	–	Nat. Acad. Sci. 1972 Kaden et al. 1979
1-Methylcarbazole	–		La Voie et al. 1982
2-Methylcarbazole	–		La Voie et al. 1982
3-Methylcarbazole	–		La Voie et al. 1982
4-Methylcarbazole	–		La Voie et al. 1982
9-Methylcarbazole	+		La Voie et al. 1982
1,9-Dimethylcarbazole	–		La Voie et al. 1982
2,9-Dimethylcarbazole	+		La Voie et al. 1982
3,9-Dimethylcarbazole	+		La Voie et al. 1982
4,9-Dimethylcarbazole	+		La Voie et al. 1982
9-Ethylcarbazole	+		La Voie et al. 1982
9-Isopropylcarbazole	–		La Voie et al. 1982
9-Benzylcarbazole	–		La Voie et al. 1982
9-Phenylcarbazole	–		La Voie et al. 1982
9-Hydroxymethylcarbazole	+		La Voie et al. 1982
9-Formylcarbazole	–		La Voie et al. 1982
9-Acetylcarbazole	–		La Voie et al. 1982
1-Aminoanthracene	+	+	McCann et al. 1975
2-Aminoanthracene	+	+	McCann et al. 1975
9-Aminoanthracene	+		Lee and Castle 1981
2-Aminoflorene	+	+	McCann et al. 1975
<u>4-ring</u>			
1-Nitrofluoranthene	+		Klopman and Rosenkranz 1984
3-Nitrofluoranthene	+		Klopman and Rosenkranz 1984

continued...

Table 12. Continued.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
7-Nitrofluoranthene	+		Klopman and Rosenkranz 1984
8-Nitrofluoranthene	+		Klopman and Rosenkranz 1984
2-Nitrochrysene	-		Klopman and Rosenkranz 1984
5-Nitrochrysene	-		Klopman and Rosenkranz 1984
6-Nitrochrysene	+		Klopman and Rosenkranz 1984
1-Nitropyrene	+	+	Rosenkranz 1984 Klopman and Rosenkranz 1984
2-Nitropyrene	+		Klopman and Rosenkranz 1984
1,3-Dinitropyrene	+	+	Rosenkranz 1984 Klopman and Rosenkranz 1984
1,6-Dinitropyrene	+	+	Rosenkranz 1984 Klopman and Rosenkranz 1984
1,8-Dinitropyrene	+	+	Rosenkranz 1984 Klopman and Rosenkranz 1984
1,3,6-Trinitropyrene	+		Klopman and Rosenkranz 1984
1,3,6,8-Tetranitropyrene	+		Klopman and Rosenkranz 1984
3-Hydroxy-1-nitropyrene	+		Ball et al. 1984
8-Hydroxy-1-nitropyrene	+		Ball et al. 1984
6+8-Hydroxy-1-nitropyrene	+		Ball et al. 1984
6-Hydroxy-1-nitropyrene	+		Ball et al. 1984
6-Nitrobenzo(a)anthracene	-		Klopman and Rosenkranz 1984
7-Nitrobenzo(a)anthracene	-		Klopman and Rosenkranz 1984
Dimethylnitrosamine	+	+	DeFlora et al. 1984
6-Aminochrysene	+	+	McCann et al. 1975
Benzo(a)carbazole	+	+	Nat. Acad. Sci. 1972 Dipple 1976
Benzacridine	-	+	Rinkus and Legator 1979 Kimball and Munro 1981
7,9-Dimethylbenz(c)acridine	+	+	McCann et al. 1975
7,10-Dimethylbenz(c)acridine	+	+	Rinkus and Legator 1979

continued...

Table 12. Concluded.

Compound	Mutagenic Activity	Carcinogenic Activity	Reference
1-Aminopyrene	+		Ball et al. 1984
3-Aminopyrene	+		Guerin et al. 1980
N-Acetyl-1-aminopyrene	+		Ball et al. 1984
N-Hydroxyl-N-acetyl-1-aminopyrene	+		Ball et al. 1984
3-,6-,8-Hydroxyl-nitropyrene (mixture)	+		Ball et al. 1984
5-ring			
1-Nitrobenzo(e)pyrene	+		Klopman and Rosenkranz 1984
3-Nitrobenzo(e)pyrene	+		Klopman and Rosenkranz 1984
6-Nitrobenzo(a)pyrene	+		Pitts, Jr. et al. 1982
3-Nitroperylene	+		Klopman and Rosenkranz 1984
3-Aminoperylene	+	+	Guerin et al. 1980
Dibenz(a,j)acridine	+	+	McCann et al. 1975
Dibenz(a,h)acridine	+	+	Helmes et al. 1982
Dibenz(c,h)acridine		+	Nat. Acad. Sci. 1972
Dibenzo(a,g)carbazole	+	+	Nat. Acad. Sci. 1972 Dipple 1976
Dibenzo(c,g)carbazole	+	+	Nat. Acad. Sci. 1972 Dipple 1976
Dibenzo(a,i)carbazole	+	+	Nat. Acad. Sci. 1972 Dipple 1976
7H-Benzo(a)pyrido(2,3-a)carbazole		+	Dipple 1976
7H-Benzo(a)pyrido(3,2-a)carbazole		+	Dipple 1976
6-rings			
7-Nitrobenzo(g,h,i)perylene	-		Klopman and Rosenkranz 1984

+ = mutagenic or carcinogenic activity
- = no mutagenic or carcinogenic activity detected

Table 13. Mutagenic activity of sulphur compounds.

Compound	Mutagenic Activity	Reference
<u>3-rings</u>		
Dibenzothiophene	-	McFall et al. 1984
1-Methyldibenzothiophene	-	McFall et al. 1984
2-Methyldibenzothiophene	-	McFall et al. 1984
3-Methyldibenzothiophene	-	McFall et al. 1984
4-Methyldibenzothiophene	-	McFall et al. 1984
Naphtho(2,3-b)thiophene	-	Lee and Castle 1981
Naphtho(2,1-b)thiophene	-	Lee and Castle 1981
Naphtho(1,2-b)thiophene	+	Lee and Castle 1981
Anthra(1,2-b)thiophene	+	Lee and Castle 1981
Anthra(2,1-b)thiophene	+	Lee and Castle 1981
<u>4-rings</u>		
Phenanthro(2,3-b)thiophene	-	Lee and Castle 1981
Phenanthro(3,2-b)thiophene	-	Lee and Castle 1981
Phenanthro(1,2-b)thiophene	-	Lee and Castle 1981
Phenanthro(2,1-b)thiophene	-	Lee and Castle 1981
Phenanthro(3,4-b)thiophene	+	Lee and Castle 1981
Phenanthro((4,3-b)thiophene	-	Lee and Castle 1981
Phenanthro(9,10-b)thiophene	-	Lee and Castle 1981
Benzo(b)naphtho(2,1-d)thiophene	-	Lee and Castle 1981
1-Methylnaphtho(2,1-d)thiophene	+	McFall et al. 1984
2-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984
3-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984
4-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984
5-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984
6-Methylnaphtho(2,1-d)thiophene	+	McFall et al. 1984
7-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984
8-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984

continued...

Table 13. Concluded.

Compound	Mutagenic Activity	Reference
9-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984
10-Methylnaphtho(2,1-d)thiophene	-	McFall et al. 1984
Benzo(b)naphtho(2,3-d)thiophene	-	Lee and Castle 1981
1-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
2-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
3-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
4-Methylnaphtho(2,3-d)thiophene	+	McFall et al. 1984
6-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
7-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
8-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
9-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
10-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
11-Methylnaphtho(2,3-d)thiophene	-	McFall et al. 1984
Benzo(b)naphto(1,2-d)thiophene	-	Lee and Castle 1981
1-Methylnaphtho(1,2-d)thiophene	+	McFall et al. 1984
2-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984
3-Methylnaphtho(1,2-d)thiophene	+	McFall et al. 1984
4-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984
5-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984
6-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984
8-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984
9-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984
10-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984
11-Methylnaphtho(1,2-d)thiophene	-	McFall et al. 1984

+ = mutagenic or carcinogenic activity
- = no mutagenic or carcinogenic activity

and 2 µg/g, respectively. Although carcinogenic isomers were believed to be present among the multitude of compounds, they could not be identified with certainty. Based only on the relative abundances of these components, mutagenic activity exhibited by the aromatic portions of these oils would be caused predominantly by compounds of mass 252 or less.

The GP26 (May) sample was further separated into 29 fractions by chromatography on alumina. Each fraction was examined by synchronous fluorescence spectroscopy and fractions with similar spectra were combined. The resulting seven fractions were analysed by GC-MS and tested for mutagenicity.

The GC-MS results are summarized in Table 14.

The first aromatic fraction eluted from the column with toluene consisted mainly of alkyl substituted compounds in the mass range 178 to 234. These were primarily alkyl substituted phenanthrenes and fluorenes with up to five substituent carbon atoms. Included were compounds up to a molecular weight of 276. These higher molecular weight compounds were also highly alkyl substituted. No methyl substituted aromatic hydrocarbons of mass 242, which might indicate carcinogenic methyl chrysene isomers, were found nor were any carcinogenic or mutagenic compounds of mass 228, 252, 276, or 278.

In addition to aromatic hydrocarbons, the sample contained cyclic sulphur compounds: naphthobenzothiophenes of mass 234, methyl-naphthobenzothiophenes of mass 248, and C2-naphthobenzothiophenes of mass 262. These sulphur compounds represented about 9% of the total sample.

The cyclic sulphur compounds were the major components of the second aromatic fraction, 98-67-35. The most abundant compound was a naphthobenzothiophene, with C1-, C2-, and C3-naphthobenzothiophenes all being major constituents. These cyclic compounds accounted for 41% of the sample. The aromatic hydrocarbons consisted of alkyl substituted fluorenes, phenanthrenes, fluoranthenes, benzofluorenes, and pyrenes. In addition, methyl substituted aromatic hydrocarbons, including methyl chrysenes, some of which may have been carcinogenic, were present as were benz(a)anthracene and chrysene, compounds which are weakly mutagenic, were also present. No carcinogenic compounds of mass 252, 276, 278, or 302 were detected.

Table 14. Aromatic hydrocarbons in GP26 (May) oil. (Percent composition of aromatic fraction based upon the molecular ion response.)

Compound Type/ Molecular Ions	Fraction Number 1 (98-67-36)	2 (98-67-35)	3 (98-67-34)	4 (98-67-33)	5 (98-67-32)	6 (98-67-31)	7 (98-67-30)
fluorenes 166, 180, 194, 208, 222	11.3	7.9	2.6	ND	ND	ND	ND
phenanthrenes, anthracenes 178, 192, 206, 220, 234	39.9	19.0	6.2	3.1	1.5	ND	ND
fluoranthenes, pyrenes, benzofluorenes 202, 216, 230, 244, 258, 272, 286	11.7	21.7	18.9	25.6	25.9	14.8	42.5
chrysenes, triphenylenes, benz(a)anthracenes 228, 242, 256, 270, 284, 298	ND	4.3	43.3	45.4	31.4	ND	ND
benzo(ghi)fluoranthene 226	ND	0.5	ND	ND	ND	ND	ND
binaphthyl 254	ND	1.8	ND	ND	ND	ND	
benzofluoranthenes 252	ND	ND	ND	0.4	3.4	12.0	
benzo(e)pyrene 252	ND	ND	ND	2.0	4.6	ND	ND
benzo(a)pyrene 252	ND	ND	ND	1.0	2.7	ND	ND

continued...

Table 14. Concluded.

Compound Type/ Molecular Ions	Fraction Number 1 (98-67-36)	2 (98-67-35)	3 (98-67-34)	4 (98-67-33)	5 (98-67-32)	6 (98-67-31)	7 (98-67-30)
perylene 252	ND	ND	ND	1.0	3.9	ND	ND
alkylated compounds 266, 280, 294	ND	ND	ND	1.0	14.9	30.5	8.4
alkylated compounds 276, 290, 304	ND	ND	ND	ND	2.0	15.0	42.3
alkylated compounds 278, 292	ND	ND	ND	ND	0.3	10.0	6.9
dibenzopyrene 302	ND	ND	ND	ND	0.5	ND	ND
Sulphur Compounds							
naphthabenzothiophenes 234, 248, 262	2.6	40.6	22.1	9.9	ND	ND	ND

ND = non-detectable

The third aromatic fraction, 98-67-34, was dominated by the occurrence of benz(a)anthracene and chrysene and the C1-, C2-, and C3-substituted analogues. These compounds, many of which are mutagenic, constituted about 40% of the sample. Next in order of abundance were C1- and C2-substituted fluoranthenes and pyrenes followed by the cyclic sulphur compounds of mass 234, 248, 262, and 276. No carcinogenic hydrocarbons of mass 252, 276, 278, or 302 were detected.

The fourth aromatic fraction was also dominated by the presence of benz(a)anthracene and chrysene and the C1-, C2-, C3-substituted compounds. These represented about 45% of the sample. Next in abundance were the alkyl substituted fluoranthenes and pyrenes. Cyclic sulphur compounds were present but were far less abundant than in the previous fractions. Benzo(e)pyrene, benzo(a)pyrene, and perylene were also present. Although not as abundant as the substituted anthracenes and chrysenes, the well-known carcinogen benzo(a)pyrene, mass 252, was present to the extent of 9% of the major compound, chrysene. Also found were compounds of mass 266 indicative of methyl substituted 252 compounds. Several of these may be carcinogenic.

The major components in the fifth aromatic fraction, 98-67-32, were benzo(e)pyrene, benzo(a)pyrene, and benzofluoranthenes. Benzo(a)-pyrene is carcinogenic as are some benzofluoranthene isomers. Also present were possible carcinogenic compounds of mass 242, 256, and 266. A single cyclic ketone of mass 194 was detected in small quantities in this fraction.

The sixth aromatic fraction contained many compounds of mass 252 to mass 298. These included compounds of mass 276 and 278 which may be carcinogenic. Compounds of mass 228 and 242 were not found.

The seventh aromatic fraction, 98-67-30, contained aromatic compounds of mass 244 to 316. Included were compounds of mass 266, 276, 290, 278, and 292 which may be carcinogenic. Also found were compounds of mass 302 and 316, indicative of dibenzopyrenes and methyl dibenzopyrenes, several isomers of which are carcinogenic. Although absolute comparisons cannot be made, the high molecular weight compounds found in fractions 98-67-31 and 98-67-30 were in low concentrations as compared with the abundant alkyl aromatic hydrocarbons found in earlier fractions from the alumina column.

3.2.3 UMATAC Oils

Oils produced by the UMATAC retorting process have undergone rigorous thermal treatment. As a consequence they contain numerous low molecular weight aromatic hydrocarbons and aromatic sulphur compounds which are not found in untreated Athabasca bitumen. Analytical results for the UMATAC oils are summarized in Table 15 and are presented in Tables 6.6.1 to 6.6.5, Appendix 6. The extraction process used in this project to separate high molecular weight aromatic hydrocarbons from oils may result in losses of these lower molecular weight compounds. Despite these possible losses, naphthalene and its alkylated homologues in the molecular weight range of 128 to 170 were the most abundant aromatic compounds found, totalling 6232 ppm in an overhead oil sample. Next in order of abundance were benzothiophene and its alkyl substituted analogues in the molecular weight range 134 to 204, totalling 4941 ppm. The sulphur bearing aromatic compounds were generated by the cracking of the heavy Athabasca bitumen which has a sulphur content of about 5%. Alkyl substituted fluorenes were the next in abundance totalling 638 ppm. A second overhead oil sample showed a similar array of compounds but with greater losses of the lower molecular weight compounds (Table 6.6.2).

Of interest was the presence of acenapthene and acenaphthylene, two compounds which are on the US Environmental Protection Agency's list of priority pollutants. Other compounds on the priority pollutant list which were found in the UMATAC overhead vent oil were anthracene, benzo(a)anthracene, benzofluoranthenes, benzo(a)pyrene, benzo(ghi)perylene, chrysene, fluoranthene, fluorene, naphthalene, phenathrene, and pyrene. Known carcinogens and mutagens such as benzo(a)pyrene, benzo(e)pyrene, perylene, and benzofluoranthenes were present but only in small quantities of 1.2 to 3.2 ppm. These concentrations are in the range found in most crude oils.

The UMATAC sidedraw oil contained a wide array of aromatic compounds including not only hydrocarbons but also many heterocyclic sulphur and nitrogen compounds. The aromatic compounds previously identified in the overhead oil were also found in the sidedraw oil, Table 6.6.3. Major hydrocarbon constituents were: alkyl substituted

Table 15. Polycyclic aromatic hydrocarbons in oils from the UMATAC project and from combustion tube experiments (μg/g of original oil).

UMATAC Compound Type Molecular Ions	UMATAC Overhead Oil	UMATAC Overhead Oil	UMATAC Sidedraw Oil	Combustion Tube Oil 159-11	Combustion Tube Oil 159-14
naphthalenes 128, 142, 156, 170	6232	2365	2172	479	488
benzothiophenes 134, 148, 162, 176, 190, 204	4941	3371	2079	486	514
fluorenes 166, 180, 194, 208, 222	638	535	1167	47	84
phenanthrenes, anthracenes 178, 192, 206, 220, 234	475	680	3355	519	478
dibenzothiophenes 184, 198, 212, 226, 240	593	741	4064	590	680
fluoranthenes, pyrenes benzofluorenes, 202, 216, 230, 244, 258, 272, 286	67	27	1146	293	222
chrysenes, triphenylenes benzo(a)anthracene, 228, 242, 256, 270, 284, 298	54	ND	977	188	150
benzonaphthothiophenes 234, 248, 262, 276	63	ND	1491	306	307
benzofluoranthenes, 252	3.2	ND	24	7.5	8.1
benzo(e)pyrene 252	3.2	ND	44	2.4	9.8
benzo(a)pyrene 252	2.9	ND	32	2.6	4.2
perylene 252	1.2	ND	18	7.1	8.6
alkylated compounds 266, 280, 294	12.5	ND	14	37	29
276, 290, 304	1.1	ND	ND	ND	ND

ND = not determined

naphthalenes in the molecular weight range 142 to 184, totalling 2172 ppm; alkyl substituted phenanthrenes, m.w. 178-220, totalling 3355 ppm; and alkyl fluorenes, m.w. 166-208, totalling 1167 ppm. Many higher molecular weight aromatic hydrocarbons were present in concentrations greater than normally found in crude oils. Among these were isomers known or suspected to be carcinogenic or mutagenic. Benzo(a)-anthracene, a moderately active mutagen and carcinogen occurred at a concentration of 55 ppm. Chrysene, a carcinogen, and triphenylene, a mutagen, totalled 150 ppm. Numerous methyl and dimethyl benzo(a)-anthracenes, chrysenes, and triphenylenes of molecular weights 242 and 256 were found. These compounds totalled 772 ppm. Although specific isomers were not identified in this study, most methyl and dimethyl benzo(a)anthracene isomers are carcinogenic (Coombs et al. 1976; Dipple 1976) as are the trimethyl benzo(a)anthracenes which have been tested to date (Dipple 1976). Methyl chrysene isomers (m.w. 242) are also carcinogens or cancer initiators (Coombs et al. 1976). Pyrene, m.w. 202, was found at a concentration of 180 ppm and fluoranthene, m.w. 202, at a concentration of 91 ppm. Both compounds and some of their alkylated homologues of molecular weights 216 and 230 are carcinogenic and fluoranthene is reported to be more active than benzo(a)-pyrene (Kady et al. 1979). Also of interest are the relatively high concentrations of benzo(a)pyrene at 32 ppm and perylene at 18 ppm. Perylene is a more potent mutagen than benzo(a)pyrene (Kady et al. 1979).

The UMATAC sidedraw oil also contained numerous heteorcyclic nitrogen compounds which were formed during the retorting process. A fraction, enriched in nitrogen compounds, was obtained by the method of Lee and Castle (1981) and analysed by GC/MS. The compounds identified are listed in Table 6.6.4. The major groups of compounds were: alkylated quinolines in the molecular weight range 129 to 185, 151 ppm; alkylated carbozoles in the molecular weight range 167 to 237, 392 ppm; alkylated amino fluorenes in the molecular weight range 181 to 223, 45 ppm; alkylated benzoquinolines in the molecular weight range 195 to 221, 44 ppm; alkylated benzocinnolines in the molecular weight range 180 to 208, 77 ppm; and alkylated benzocarbazoles in the molecular weight range 231 to 245, 29 ppm. Among the compounds identified were several known or suspected carcinogens and mutagens, some in relatively high concentrations. The mutagen 1-aminopyrene (Ball et al. 1984) was present at a concentration of 51 ppm and the carcinogen 4-aminobiphenyl (Kimball and Munro 1981) at 17 ppm. Other known carcinogens (Dipple 1976; McCann et al. 1975) identified were: aminofluorene, 4.7 ppm; 2-aminoanthracene, 2.1 ppm; 3-aminofluoranthene, 1.7 ppm; and dibenzocarbazole, 1.3 ppm. Methyl aminobiphenyls (35 ppm), dimethyl aminobiphenyls (23 ppm), methyl aminofluorenes (13 ppm), and dimethyl aminofluorenes (23 ppm) were also present. Several isomers of these compounds are carcinogenic or mutagenic (Rinkus and Legator 1979). These concentrations of nitrogen heterocyclics and aromatic hydrocarbons indicate a higher carcinogenic activity than found with most crude oils.

Sulphur containing aromatic compounds were also present in high concentrations. Alkyl substituted benzothiophenes totalled 2079 ppm and alkyl substituted dibenzothiophenes totalled 3914 ppm. These compounds are not mutagenic or carcinogenic (Lee & Castle 1981; McFall et al. 1984). Benzonaphthothiophene isomers were found in concentrations totalling 202 ppm. Alkyl benzonaphthothiophenes, some of which are mutagenic (McFall et al. 1984), were abundant with 580 ppm methyl benzonaphthothiophenes and 709 ppm of other alkylated benzonaphthothiophenes.

A sample of UMATAC overhead oil contained many of the same compounds found in the sidedraw oil but in much lower concentrations. Two fractions enriched in nitrogen compounds were obtained by the method of Schmitter (1983) using hydrochloric acid treated silica gel. The first fraction, Table 6.6.5.1, contained mainly indoles, carbazoles, and benzocarbazoles, generally in concentrations of less than 1 ppm. The second fraction, Table 6.6.5.2, contained many compounds similar to those previously found in the sidedraw oil but in lower concentrations. Apparently the UMATAC process results in biologically active compounds accumulating in the sidedraw oil. A sample of oil from the day tank contained intermediate concentrations of aromatic compounds, e.g., 16 ppm benzo(a)pyrene as compared with 2.9 ppm in an overhead oil and 32 ppm in the sidedraw oil.

3.2.4 Combustion Tube Oils

Two samples of produced oil from the combustion tube experiments being carried out by the Chemical and Petroleum Engineering Department of the University of Calgary were analyzed. Both samples were taken from near the end of experiment number 159, a "dry" combustion tube experiment in which no water was injected. The results are summarized in Table 15 and presented in detail in Appendix 7, Tables 6.7.1 and 6.7.2.

The samples 159-11 and 159-14 contained a wide range of aromatic hydrocarbons and sulphur bearing aromatic compounds. Despite probable losses of the more volatile aromatic compounds, naphthalene and its alkylated homologs totalled 479 ppm in 159-11 and 488 ppm in 159-14, and low molecular weight sulphur compounds, benzothiophene and alkylated benzothiophenes, totalled 486 ppm and 614 ppm in 159-11 and 159-14, respectively. The dibenzothiophenes were the most abundant group of compounds in both samples, 590 ppm in 159-11 and 680 ppm in 159-14. The alkylated phenanthrenes and anthracenes were the second most abundant group of compounds in both samples being 519 ppm in 159-11 and 478 ppm in 159-14. Acenaphthene and other compounds found on the EPA priority pollutant list were present. These included anthracene, benz(a)anthracene, benzofluoranthenes, benzo(a)pyrene, chrysene, fluoranthene, fluorene, naphthalene, phenanthrene, and pyrene. Benzo(e)pyrene concentrations averaged 8.6 ppm, benzo(a)pyrene averaged 3.4 ppm, benzo(b)fluoranthene averaged 7.8 ppm, and perylene averaged 7.9 ppm.

Although the concentrations of aromatic hydrocarbons and aromatic sulphur compounds were greater than those found in Athabasca bitumen, they are substantially less than those found in the UMATAC produced oils which had undergone rigorous thermal treatment. The total aromatic hydrocarbons found in the combustion tube oils averaged 1600 ppm and sulphur aromatics averaged 1490 ppm. This compares with 7490 ppm aromatic hydrocarbons and 5600 ppm aromatic sulphur compounds found in a UMATAC overhead oil, and with 8950 ppm aromatic hydrocarbons and 7600 ppm aromatic sulphur compounds found in a UMATAC sidedraw oil.

3.2.5 Other Oils and Residuals

An oil and water emulsion produced from the AOSTRA-Shell project was analysed for aromatic hydrocarbons, specifically benzo(a)-pyrene. The heavy oil-water emulsion from well 44 contained 2.7 ppm benzo(a)pyrene. Because the emulsion was about 65% water, the benzo(a)pyrene content of the oil alone was 7.7 ppm. Vacuum gas oil from the diluent recovery unit contained 1.7 ppm benzo(a)pyrene, pitch from the same unit contained 1.9 ppm, and top oil contained only 0.1 ppm benzo(a)pyrene.

Refinery residuals, heavy oils, and pitches contained much higher concentrations of aromatic hydrocarbons, including benzo(a)-pyrene, than were found in any in situ produced oil or UMATAC produced oil. Catalytic cracker fractionator bottoms obtained from a refinery in Sarnia, Ontario were fractionated and the aromatic fraction analysed for benzo(a)pyrene. The benzo(a)pyrene content was high at 1050 ppm. The aromatic fraction was further separated into subfractions which were analysed for benzo(a)pyrene and tested biologically (see Section 3.3.2).

Steam cracker refinery tar also contained large amounts of benzo(a)pyrene (150 µg/g tar, or 220 µg/g of the maltene fraction of the tar). A large percentage, 55% of the maltene fraction, was soluble in DMF and, upon column chromatography on alumina, 90% of this was found to be aromatic hydrocarbons. These aromatic hydrocarbons were further fractionated into groups of compounds by chromatography on a second alumina colunn. Each subfraction was then analysed by combined gas chromatography-mass spectrometry and the mutagenicity determined by the Ames test. The total benzo(a)pyrene content of the sample was over 150 µg/g oil and some aromatic subfractions contained as much as 280 µg of BaP. Catalytic cracker heavy cycle oils contained 240 ppm benzo(a)pyrene and fluid coker heavy gas oil contained 91 ppm. These oils were also fractionated and analysed for benzo(a)pyrene content prior to biological testing.

3.3 BIOLOGICAL TESTING

3.3.1 Ames Test for Mutagenicity in Athabasca Oils

The Ames test was used to indicate mutagenic activity in the aromatic fractions of produced oils, synthetic crude oil, and refinery residuals.

Much of the introductory work on the behaviour of hydrocarbons derived from the oil sands was carried out with synthetic crude oil produced by Suncor. Of concern was the possible inability of the Ames test to effectively detect mutagenic compounds when present in complex hydrocarbon mixtures. An experiment was therefore conducted to measure the effect of the neutral fraction of synthetic crude oil (separated by ion exchange chromatography) upon the mutagenic activity of the known mutagen and carcinogen benzo(a)pyrene. Various amounts of a neutral hydrocarbon fraction from synthetic crude oil were added to solutions of benzo(a)pyrene in dimethylsulphoxide. The mutagenicity of the mixtures were compared with that of benzo(a)pyrene alone, using Salmonella strain TA98 with the addition of S9 enzymes. The addition of the oil systematically reduced the number of revertant colonies--from 328 to 73 with the addition of the equivalent of 19 mg of synthetic crude oil. Unexpectedly, the addition of more than 19 mg of the DMSO extract of synthetic crude oil resulted in an increase in the number of revertants; 112 mg gave 498 colonies (Figure 3).

The initial decrease in the number of revertant colonies with increasing amounts of synthetic crude oil could not have been caused by toxicity. Cell lethality from toxicity would have been irreversible and additional samples would have resulted in even fewer colonies. The effect of the synthetic crude oil is, therefore, thought to be the suppression of the activity of mutagens by associated hydrocarbons. This suppression may be the result of physical properties of the sample and the test system or of biological properties of the Salmonella typhimurium.

The neutral fraction of the synthetic oil was itself mutagenic with an activity of 10 revertants per mg of original oil (Figure 4). The activity in the absence of S9 was 23 revertants per mg greater than in the presence of S9 (Figure 5). This showed that direct acting

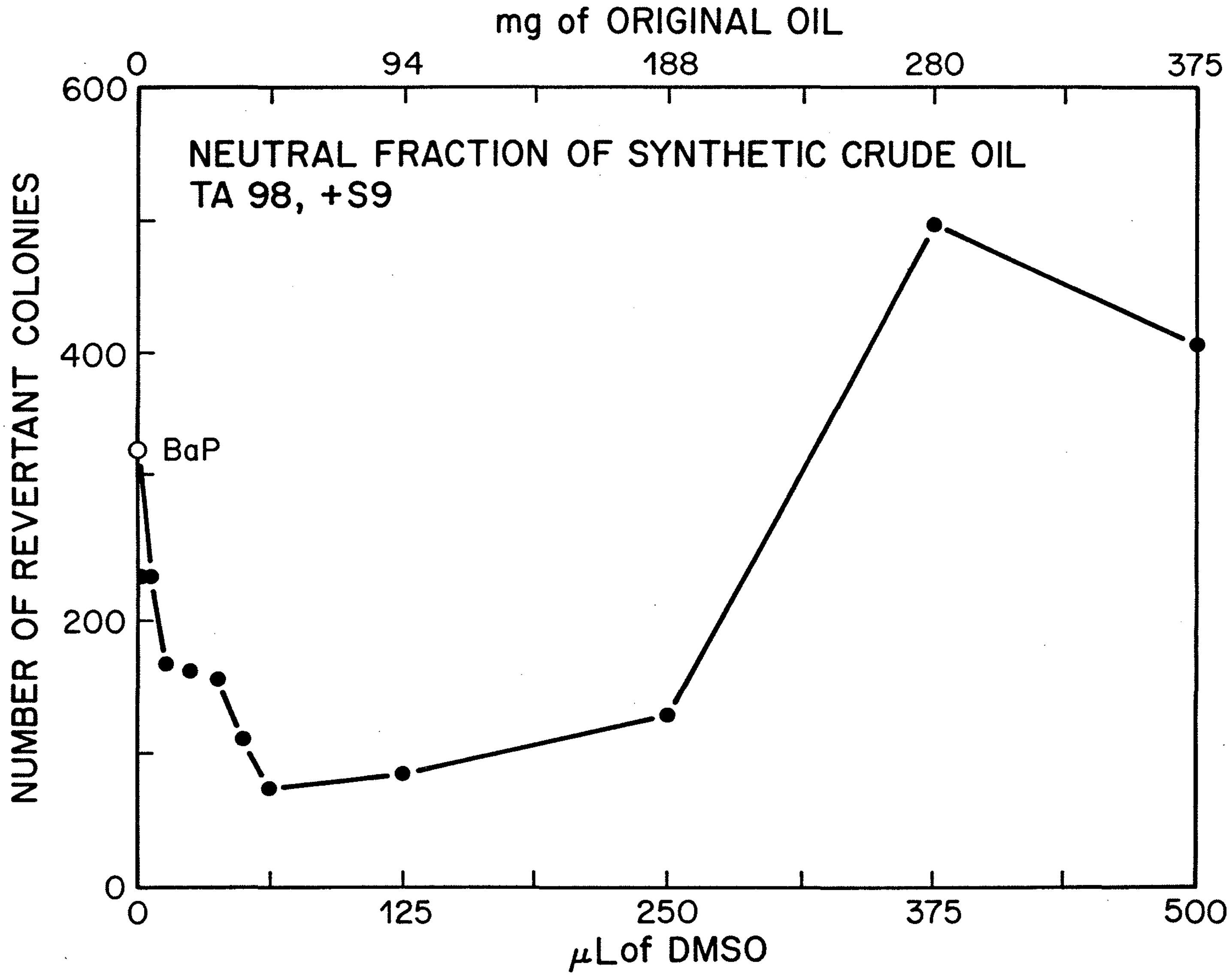

Figure 3. Ames test on synthetic crude oil with benzo(a)pyrene added.

mutagens were present and that the S9 enzymes at least partially destroyed these mutagens. Polycyclic aromatic hydrocarbons are activated by the S9 enzymes system and, therefore, the mutagenicity of the Suncor neutral fraction was caused mainly by compounds other than polycyclic aromatic hydrocarbons.

Further fractionation of the neutral fraction into "neutral nitrogen" and "neutral hydrocarbon" fractions by ferric chloride complexing demonstrated that direct acting mutagens were not confined to a single fraction of the oil as both these fractions were mutagenic (Figures 6 and 7). Multiple tests were performed on DMSO extracts of several samples of the same synthetic crude oil. The results were reproducible within a single set of analyses on a given extract (as shown by the number of revertants obtained on 3 plots at each concentration in Figures 4 and 5) but varied greatly among extracts. For example, the results presented in Figure 3 clearly show suppression of mutagenic activity to a level below that indicated by the data presented in Figure 4. This variation may reflect differences in the physical composition of each extract, the amount of dispersed hydrocarbons as distinguished from dissolved mutagens.

The effect of bitumen upon the activity of benzo(a)pyrene was tested in a manner similar to that for the synthetic crude oil. The bitumen suppressed the activity of the benzo(a)pyrene, with increasing amounts of bitumen bringing a steady decline in sample activity (Figure 8). In contrast to the results from the synthetic crude oil, no increase in the number of revertants occurred with larger amounts of bitumen. Despite the fact that benzo(a)pyrene was present, no activity was found when the neutral fraction of the bitumen was tested on strain TA98 in the presence of S9, therefore indicating suppression of activity (Figure 9).

3.3.2 Ames Test for Mutagenicity in COFCAW-Produced Oils

The foregoing Ames test results demonstrated the need for further fractionation of samples to eliminate compounds which interfere with the Ames test.

The aromatic hydrocarbons, from the oil-water emulsion collected from well GP-26 in May, were separated and fractionated as

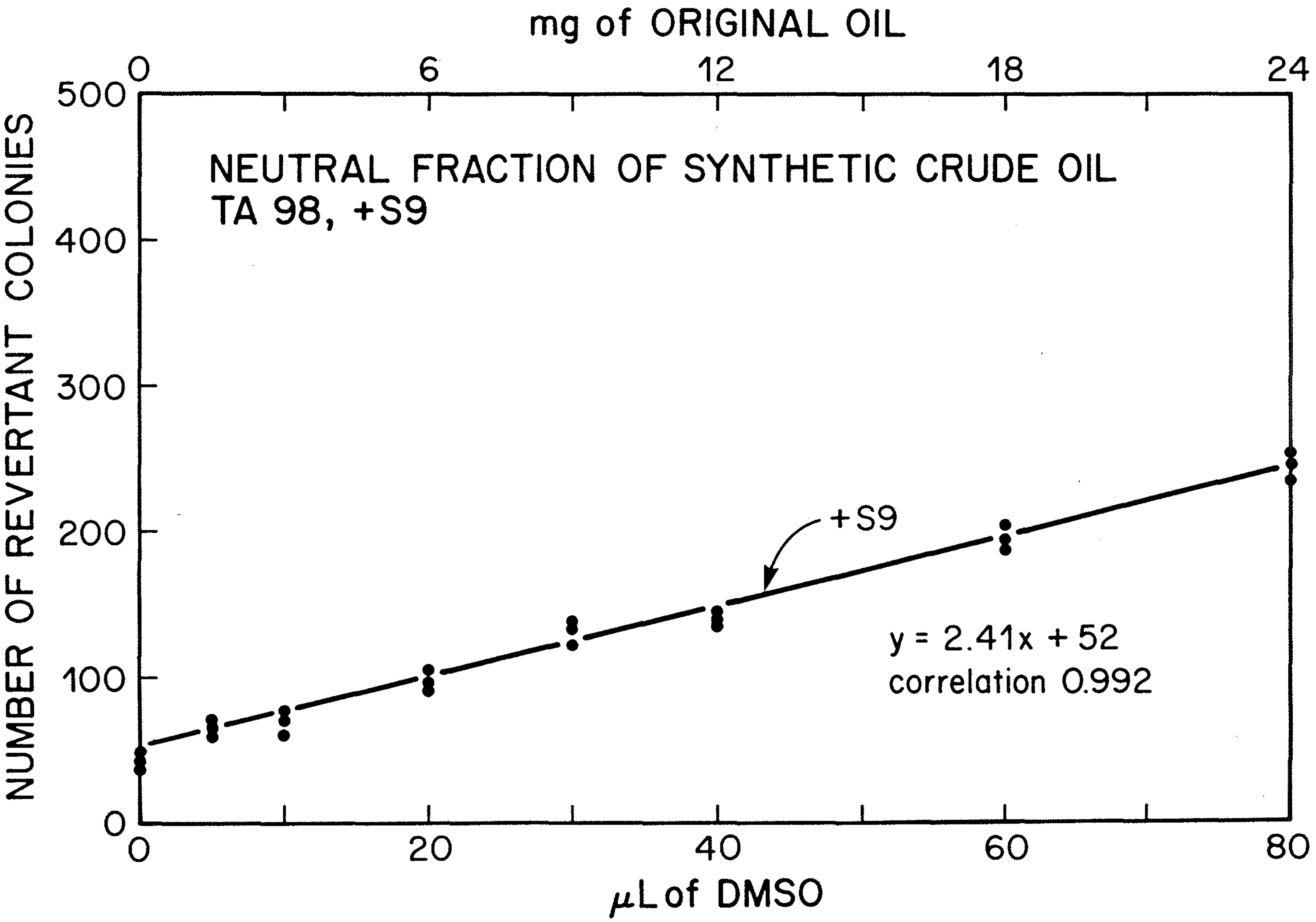

Figure 4. Ames test data on the neutral fraction of synthetic crude oil, with S9 enzymes.

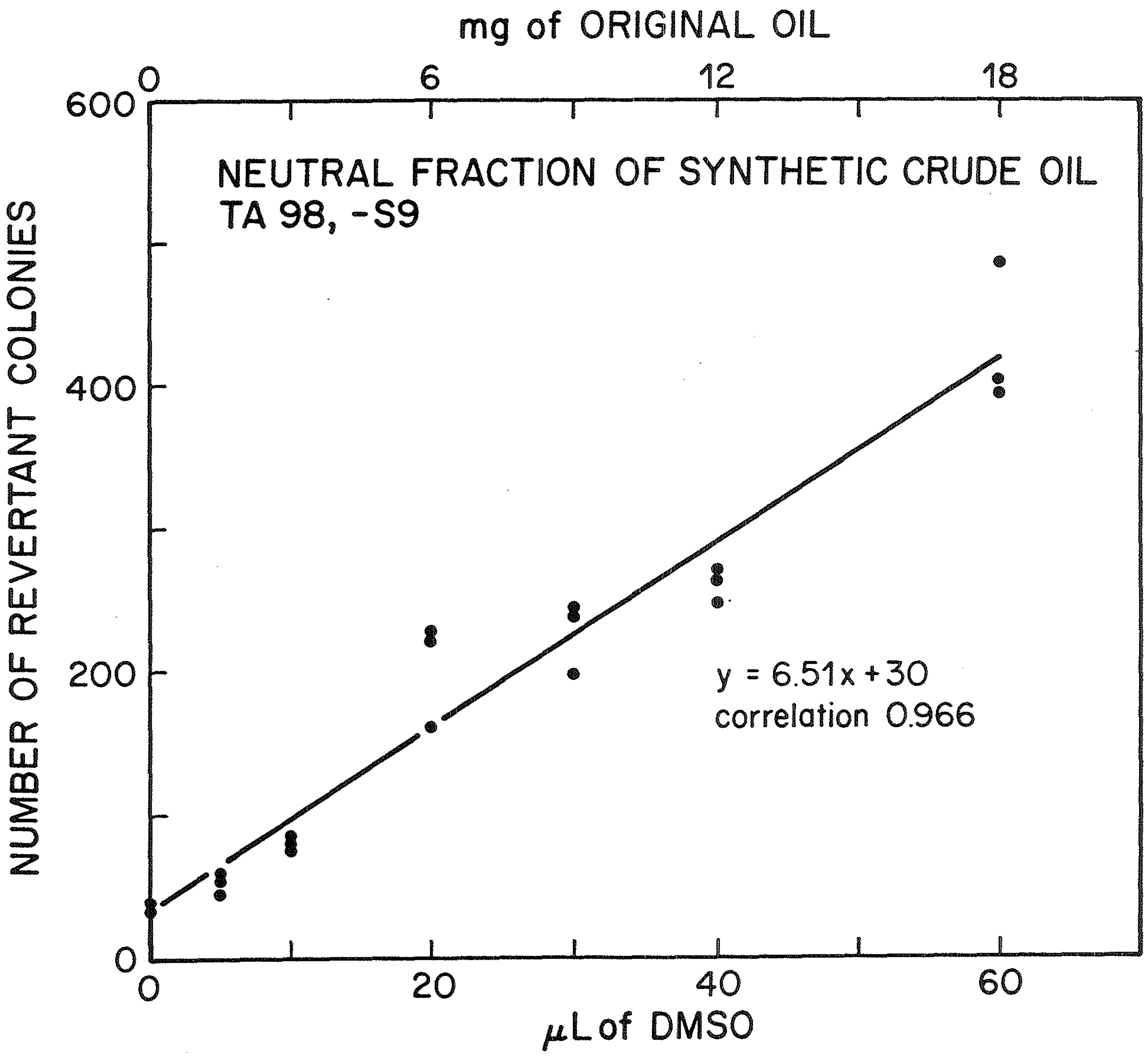

Figure 5. Ames test data for the neutral fraction of synthetic crude oil, without S9 enzymes.

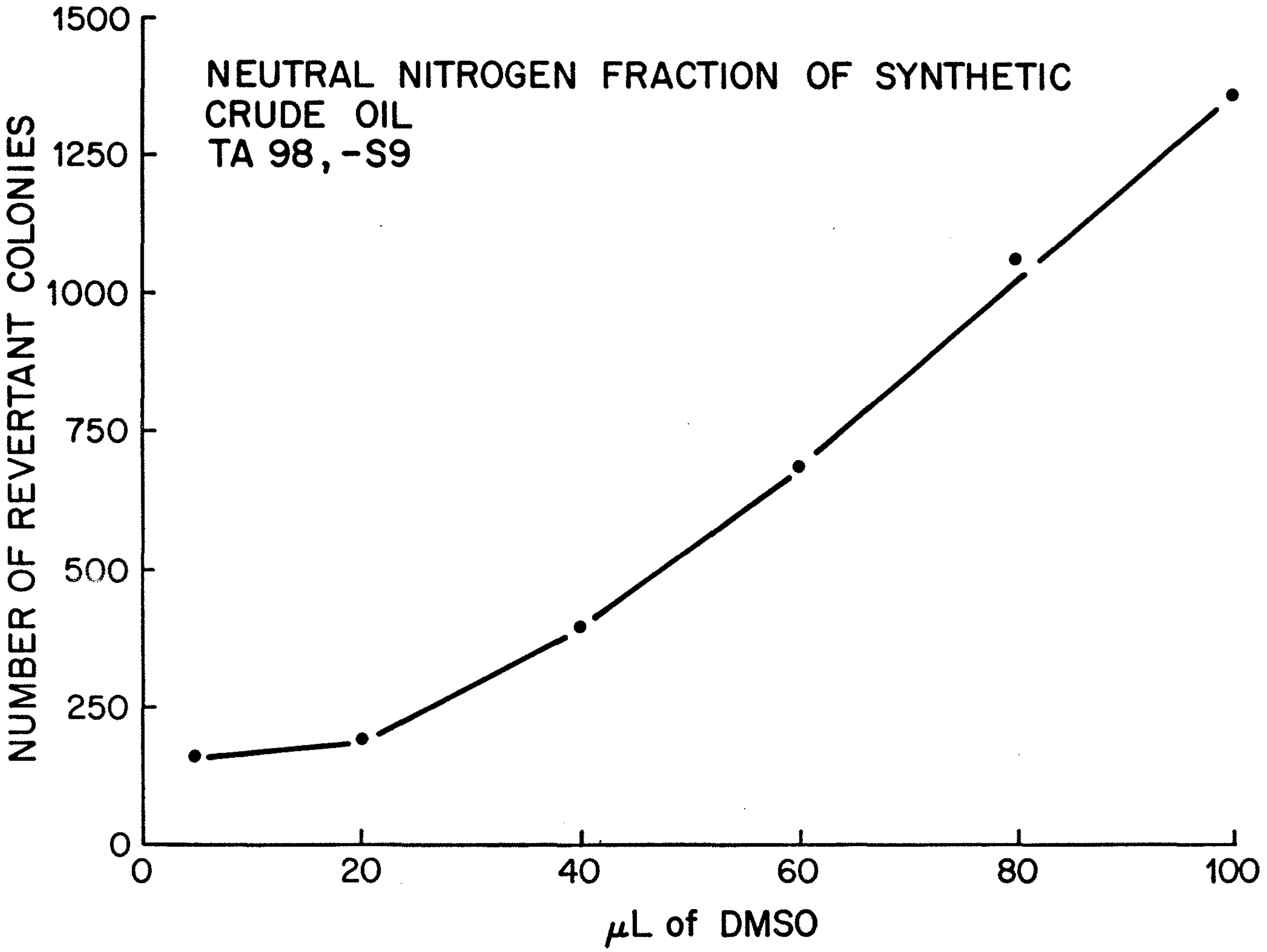

Figure 6. Ames test data for the "neutral nitrogen" components of synthetic crude oil, -S9.

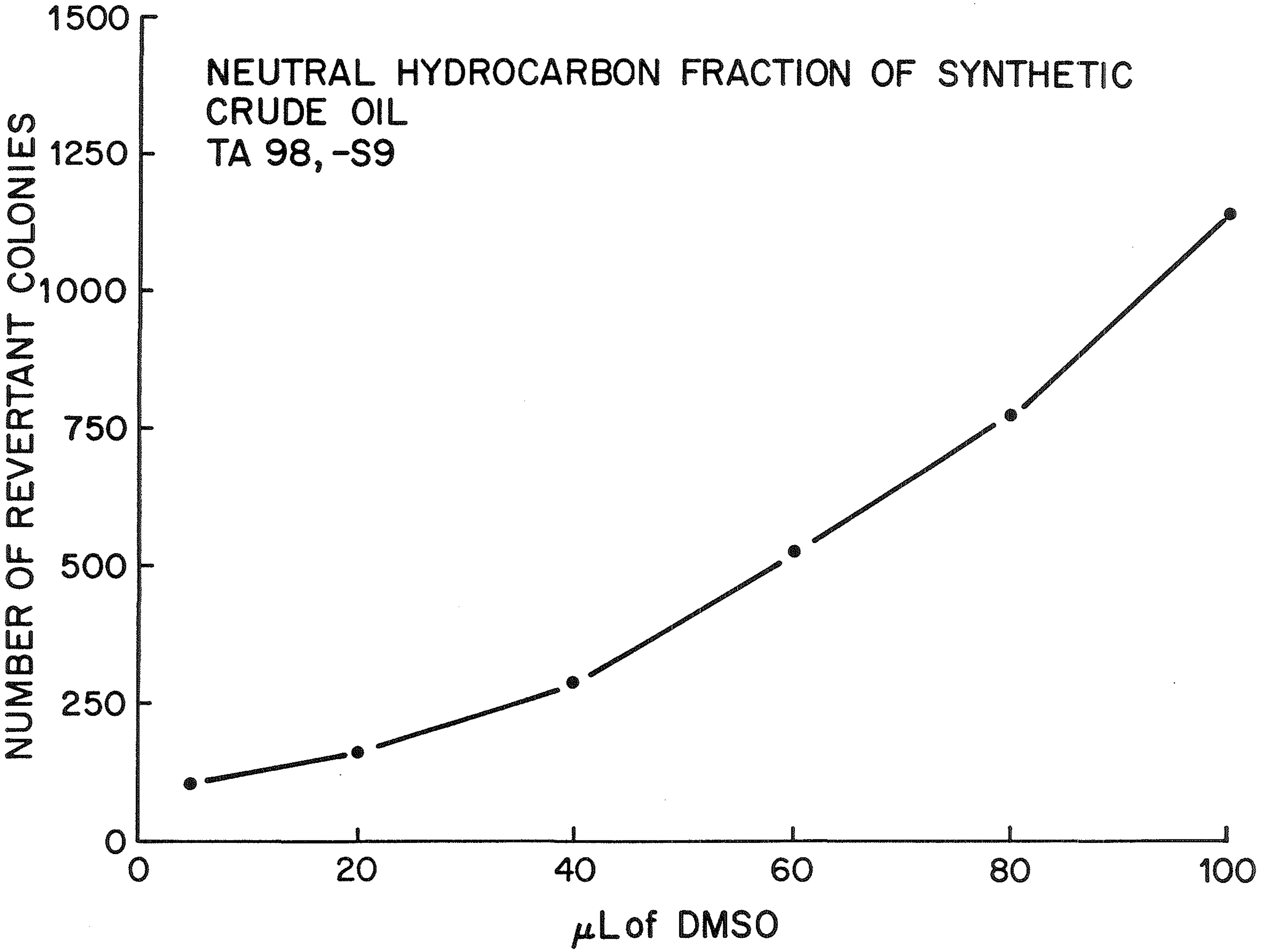

Figure 7. Ames test data for the "neutral hydrocarbon" components of synthetic crude oil, -S9.

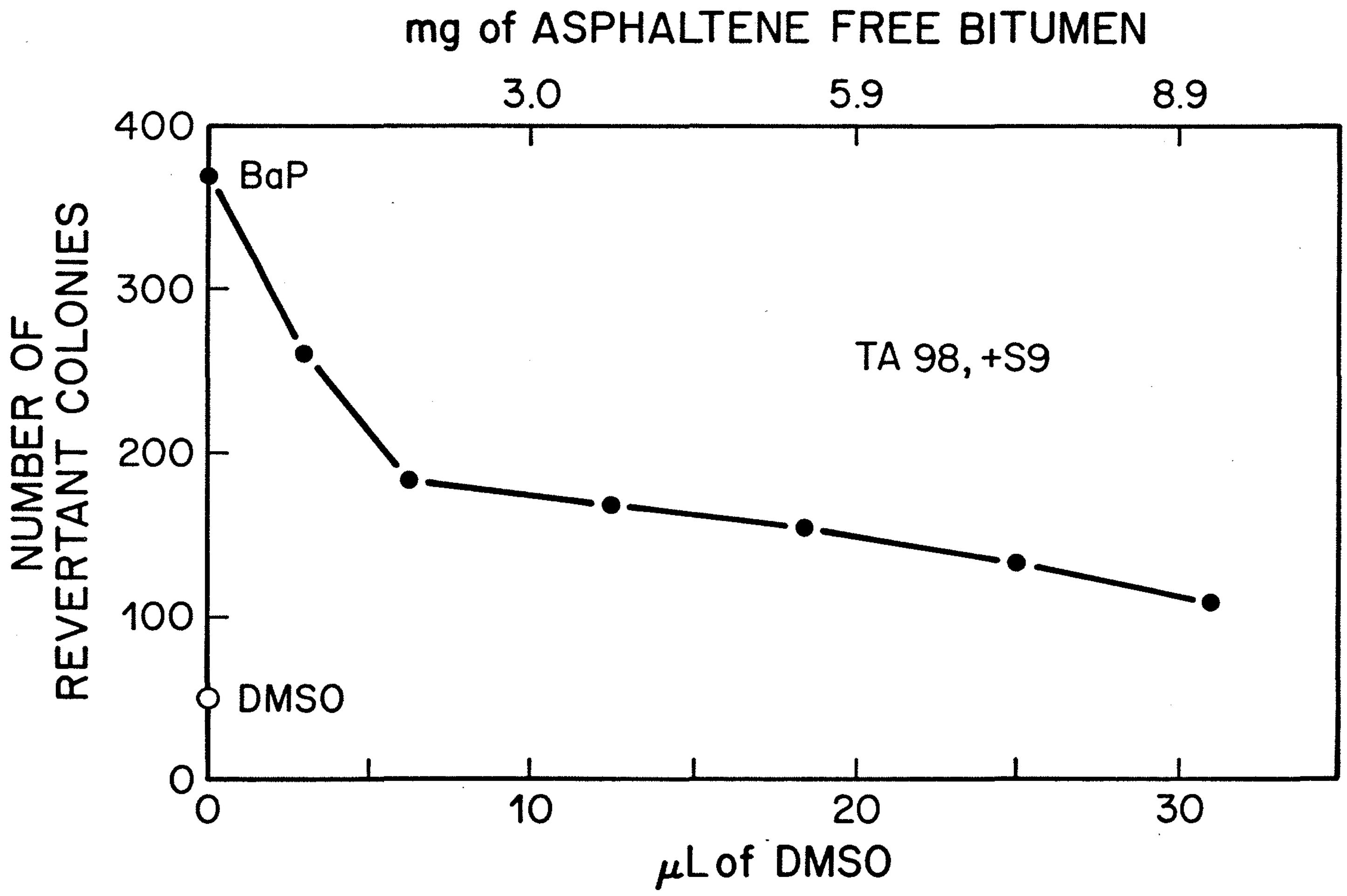

Figure 8. Ames test data for bitumen, with added benzo(a)pyrene, +S9.

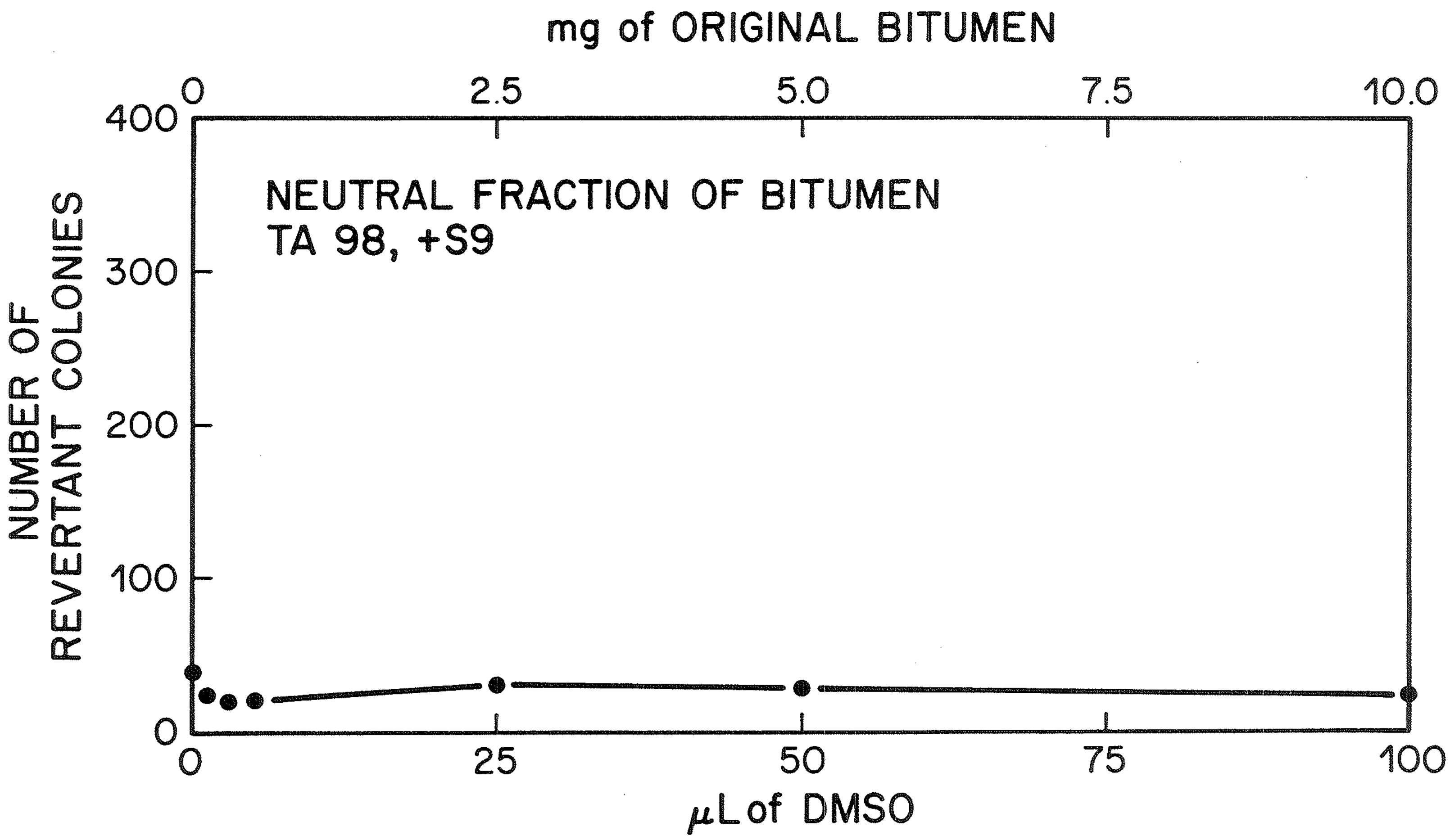

Figure 9. Ames test data for the neutral fraction of bitumen, +S9.

described in Section 2.2.3. Fractions with similar synchronous fluorescence spectra were combined, resulting in seven fractions which were analysed by GC-MS and tested for mutagenicity.

Each fraction was tested in the presence of S9 rat liver homogenate on <u>Salmonella</u> strain TA98. Two fractions (Figures 11 and 14) showed a greater than two fold increase in the number of revertants. Five of the seven fractions showed some mutagenic activity as indicated by a good correlation between the amount of sample and the number of revertants (Figures 10 to 16).

The first fraction of aromatic hydrocarbons eluted from the alumina column exhibited a mutagenic activity of 3.4 revertants per microlitre of DMSO with a very good correlation coefficient of 0.992 (Figure 10). Each sample was dissolved in an equal quantity of DMSO: thus, mutagenic activity could be compared among samples. The sample consisted largely of alkyl substituted fluorenes and phenanthrenes. Of these compounds at least five, 1-methylphenanthrene, 2-methylphenanthrene, 9-methylphenanthrene, 9-methylfluorene, and 1,9-dimethylfluorene are active in the <u>Salmonella</u> typhimurium mutagenic bio-assay. The mutagenic activity of 1,9-dimethylfluorene is reported to be twice that of benzo(a)pyrene, whereas the other compounds have mutagenicities ranging from 0.3 to 0.5 times that of benzo(a)pyrene. The alkylphenathrenes and alkylfluorenes apparently were the major mutagens present. Although an estimate of the projected mutagenic activity of the sample based solely on the abundance of these compounds could not be made, their abundance was nevertheless more than sufficient to account for the observed activity.

The second aromatic hydrocarbon fraction exhibited a mutagenic activity of 2.7 revertants per microlitre of DMSO with a correlation coefficient of 0.909 (Figure 11). In addition to alkylfluorenes and alkylphenanthrenes, the second fraction contained compounds of mass 228 and 242. Several isomers of methylchrysene, methylbenz(a)anthracene, and methylbenzo(c)phenanthrene of m/e 242 are biological active. The effect of the abundant cyclic sulphur compounds, naphthabenzothiophenes, is unknown but these compounds apparently were not sufficiently toxic to negate the test.

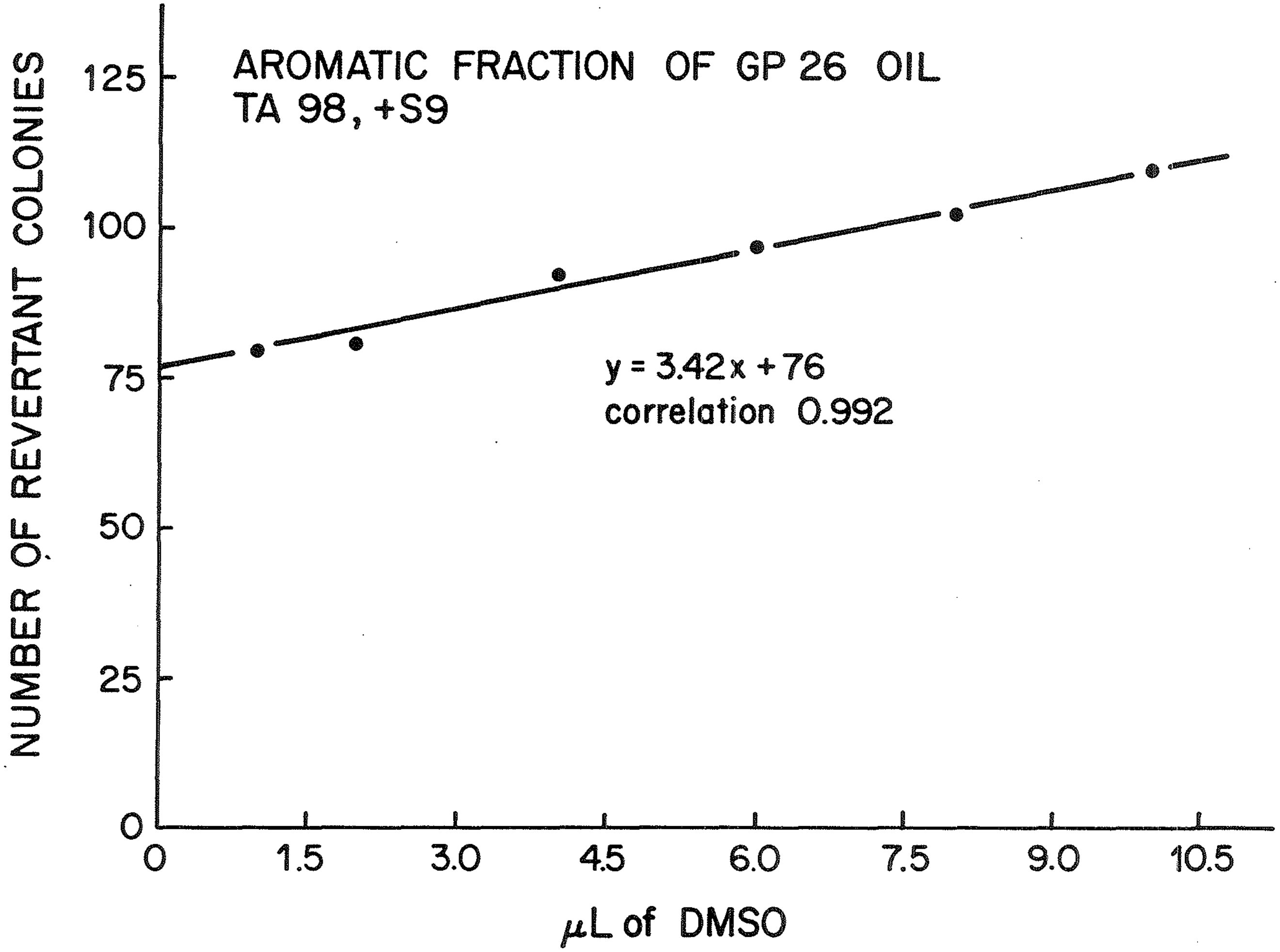

Figure 10. Ames test data for the aromatic sub-fraction 98-67-36 of GP26 oil.

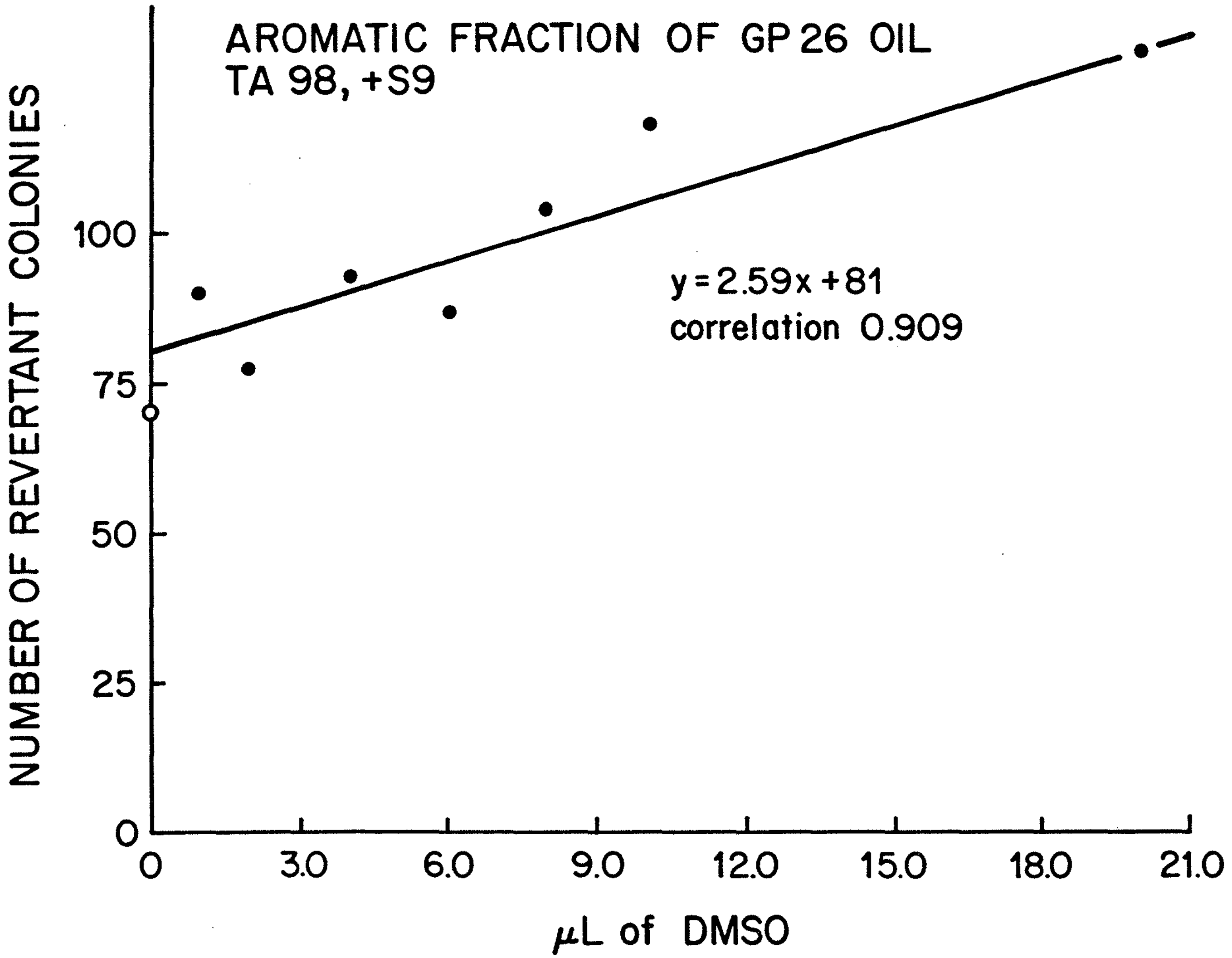

Figure 11. Ames test data for the aromatic sub-fraction 98-67-35 of GP26 oil.

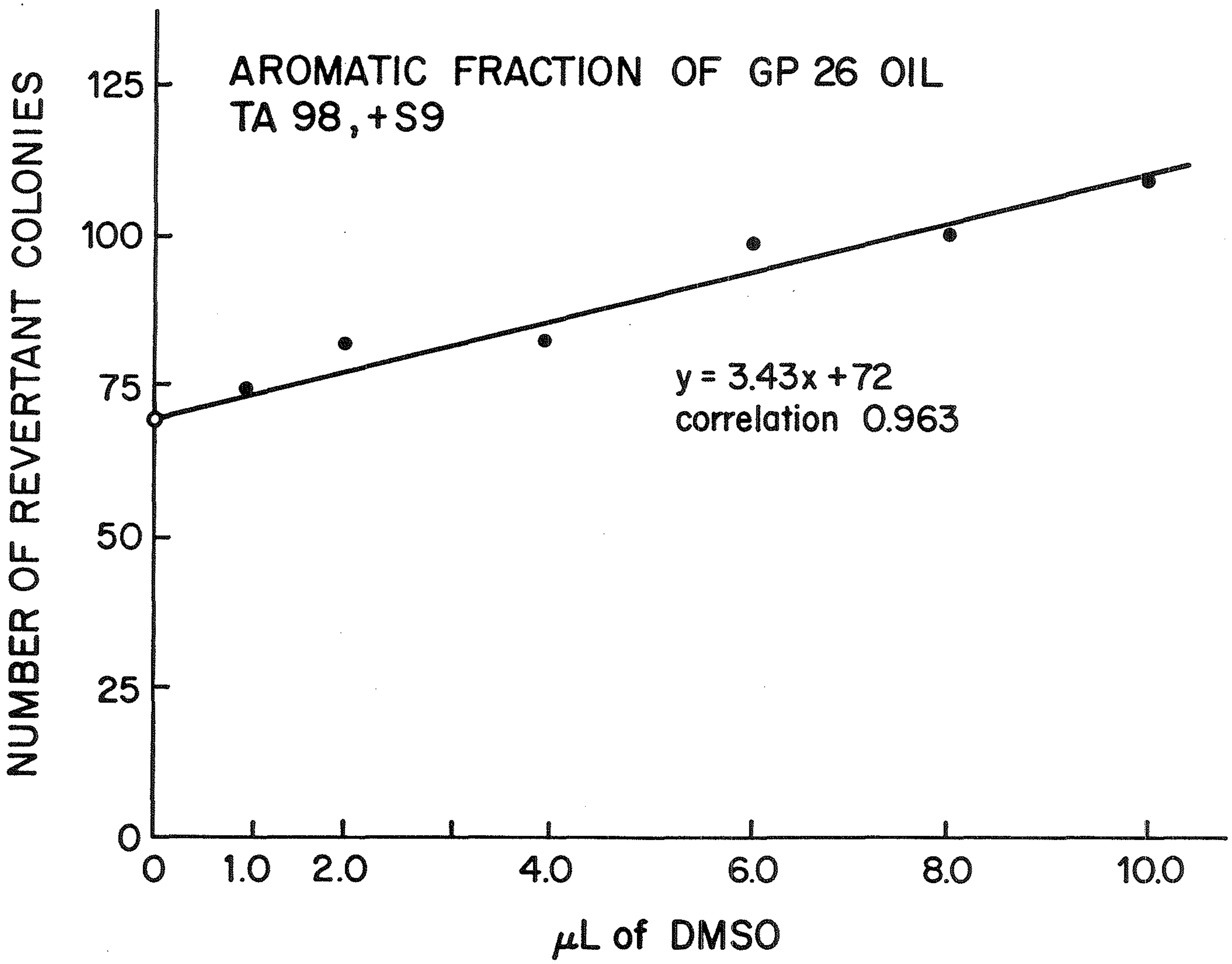

Figure 12. Ames test data for the aromatic sub-fraction 98-67-34 of GP26 oil.

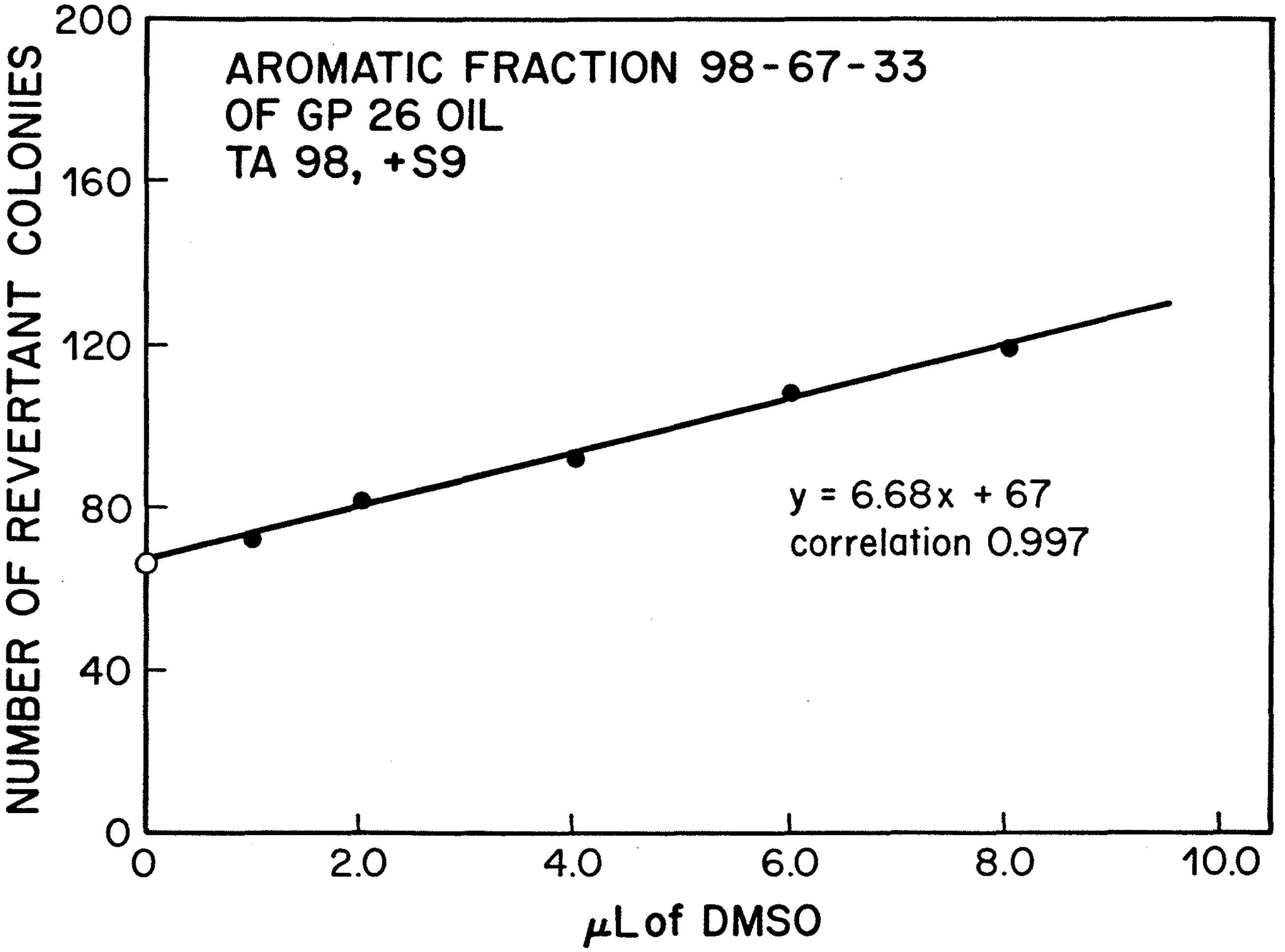

Figure 13. Ames test data for the aromatic sub-fraction 98-67-33 of GP26 oil.

The third fraction contained an abundance of mass 228, 242, and 256 compounds, many of which are mutagenic. The observed activity of 3.4 revertants per microlitre of DMSO with a correlation coefficient of 0.96 was in keeping with the presence of these known mutagens (Figure 12). When tested over a wider concentration range, the sample showed toxicity.

Fraction four was the most active with 6.7 revertants per microlitre and a correlation coefficient of 0.997 (Figure 13). This sample contained not only benz(a)anthracene, chrysene, and their mutagenic analogues, but also the carcinogen benzo(a)pyrene and benzofluoranthenes.

The fifth aromatic fraction contained 7 μg of benzo(a)pyrene as determined by combined gas chromatography-mass spectrometry. The activity was far less than would be expected from the equivalent amount of benzo(a)pyrene alone. The 7 μg of benzo(a)pyrene contained in the sample should have given in excess of 850 revertant colonies as opposed to the less than 300 colonies which were found (Figure 14). Thus, the presence of other hydrocarbons in this aromatic fraction suppressed the activity of the benzo(a)pyrene in much the same way as the activity of benzo(a)pyrene was reduced by the addition of bitumen or synthetic crude oil.

The sixth and seventh fractions from the alumina column showed slight mutagenic activity (Figures 15 and 16).

The question of whether a mixture of mutagens produces an additive effect in the Ames test has been much debated. The samples examined in this study clearly showed suppression of the activity of a mutagen caused by the presence of other hydrocarbons. This was evidenced by the decrease in mutagenic activity of benzo(a)pyrene brought about by the addition of the DMSO soluble portion of the neutral fraction of synthetic crude oil and by the less than anticipated activity of an aromatic fraction of COFCAW-produced oil which contained benzo(a)pyrene. The cause of this suppression of mutagenicity may be the physical properties of the hydrocarbon/DMSO/ aqueous system or biological properties of the Salmonella typhimurium. The mutagenic activity was lower than expected but larger amounts of sample did increase the number of revertants. This shows that the effect was not

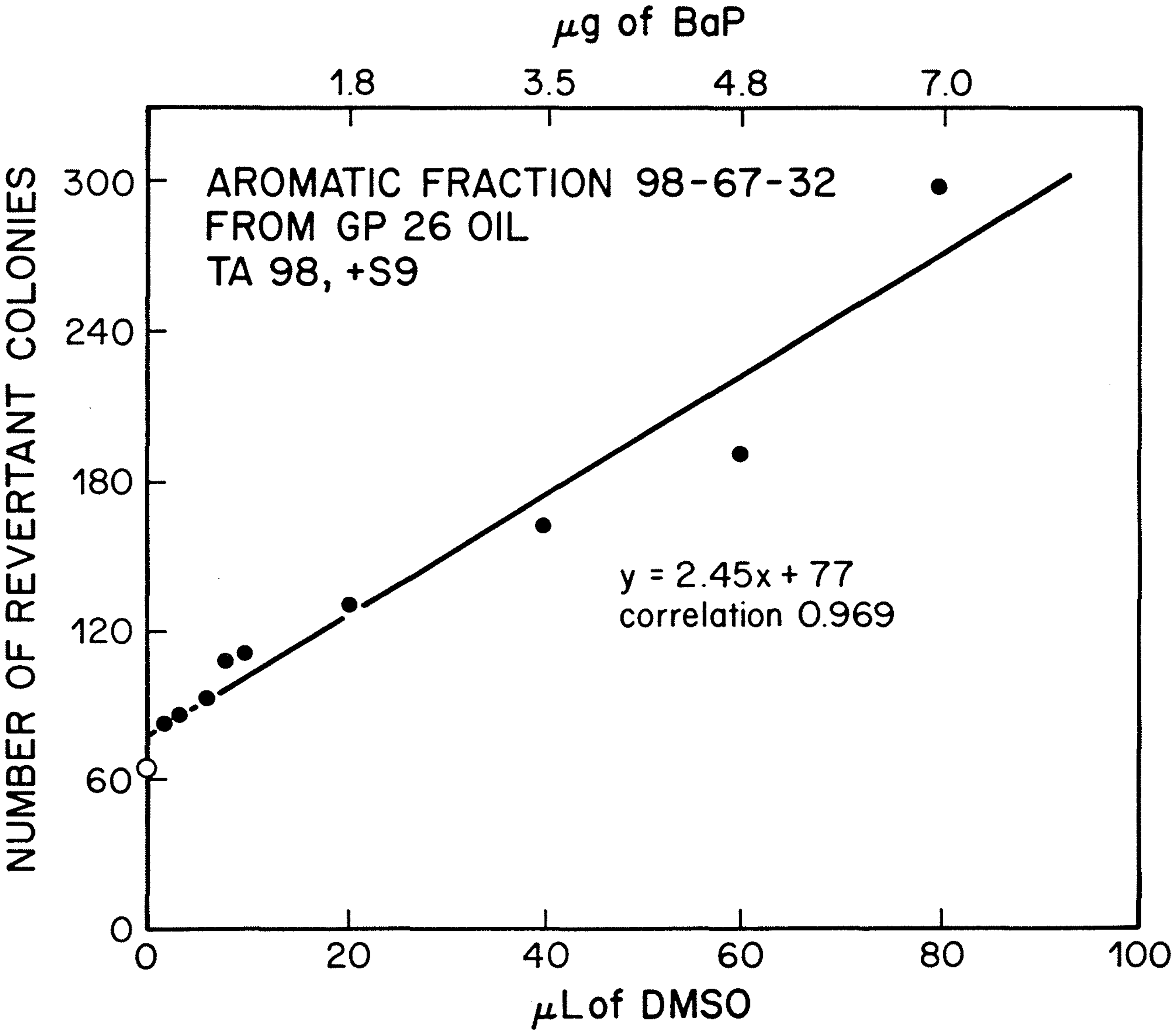

Figure 14. Ames test data for the aromatic sub-fraction 98-67-32 of GP26 oil.

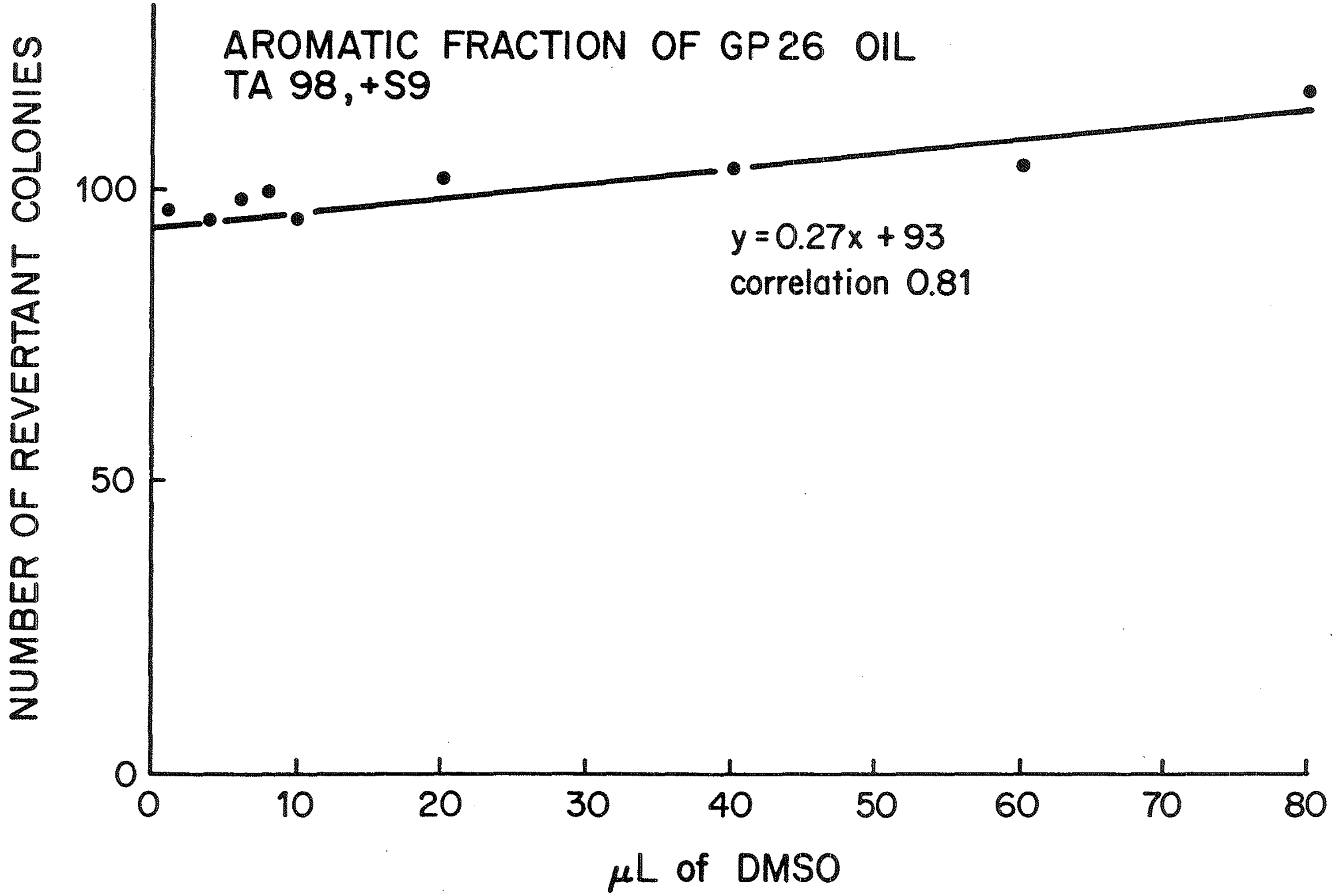

Figure 15. Ames test data for the aromatic sub-fraction 98-67-31 of GP26 oil.

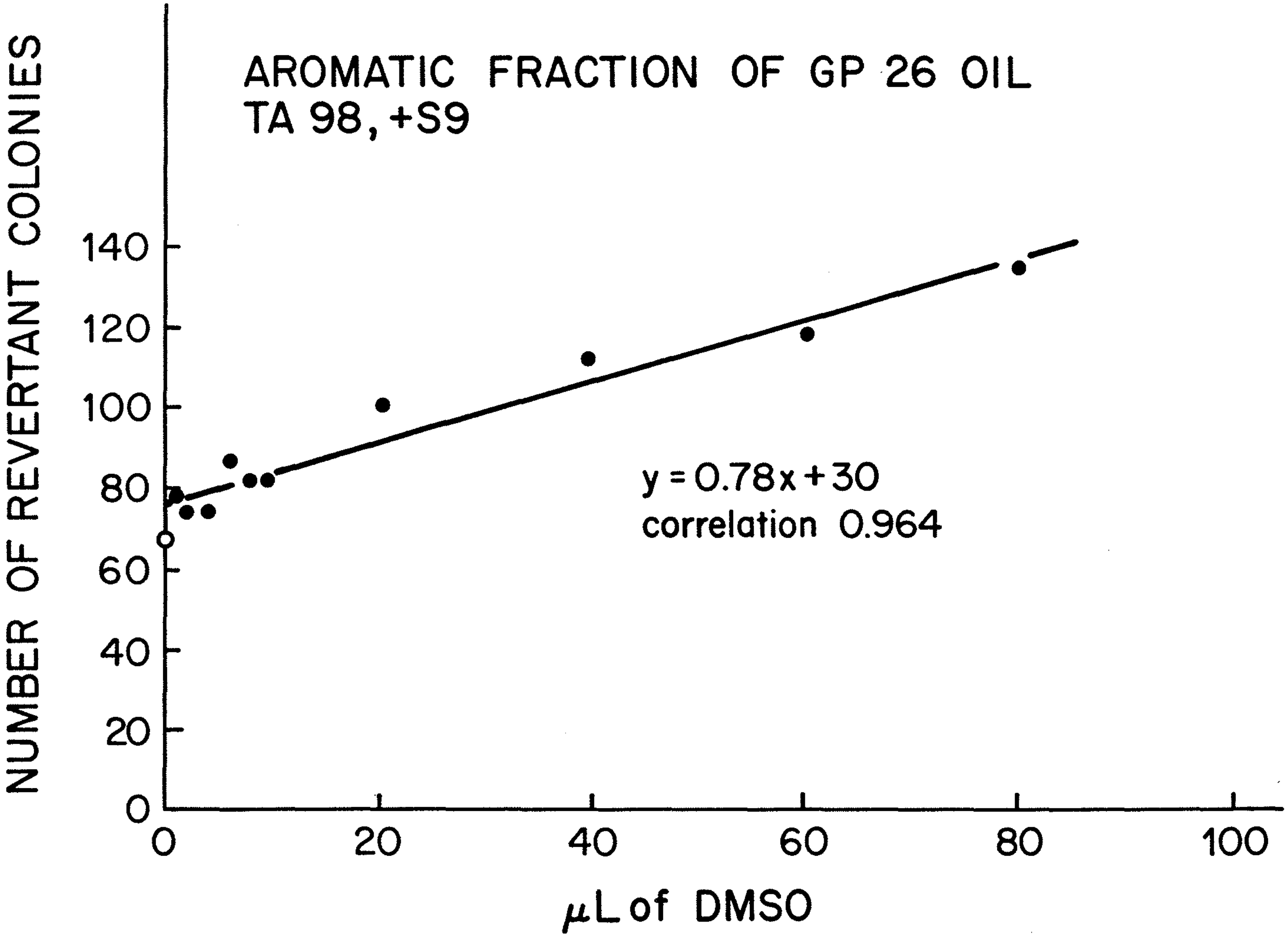

Figure 16. Ames test data for the aromatic sub-fraction 98-67-30 of GP26 oil.

caused by cell lethality which would have resulted in a continuing decline in the number of revertant colonies with increasing amounts of sample.

In view of the above findings, comparisons of the mutagenic activity of the COFCAW-produced oil with the activity of conventional crude oil, shale oil, or coal liquefaction products must be made with caution. Some fractions of the COFCAW-produced oil had mutagenic activities as high as 7400 revertants per milligram of fractionated material. These activities are higher than those reported for crude oil and shale oil fractions but less than those reported for some coal liquefaction products. The mutagenic activities of the neutral aromatic fraction and the basic fraction were approximately equal and were about ten times greater than that of the acid fraction. These fractions represent only a small proportion of the COFCAW oil and their biological behaviour in the complex organic mixture which comprises the COFCAW oil is not presently known. Their mutagenic activity as part of the whole oil may be additive, synergistic, or antagonistic. Until further information is available on the biological activity of carcinogens in complex hydrocarbon mixtures, an accurate assessment of the COFCAW-produced oil is not possible. Indications are, however, that the activity of the COFCAW oil lies between that of conventional crude oils and coal liquefaction products.

3.3.3 Ames Test for Mutagenicity of Other Oils and Refinery Residuals

3.3.3.1 SHOP Project Oils. The mutagenic activity of aromatic subfractions from heavy oils produced in the SHOP project was low, ranging from 490 to 1300 revertants per gram of oil (Table 16). The most mutagenic aromatic subfraction produced 4000 revertants per mg. This compares with values as high as 7400 revertants per mg for similar fractions from the Gregoire Lake oils produced by in-situ combustion and up to 27 000 revertants per mg for vacuum bottoms from a coal liquefaction process. Mutagenic activity was found only in the presence of S9 enzymes, demonstrating that indirect acting mutagens, such as polynuclear aromatic hydrocarbons, were dominant. Only one sample, an aromatic subfraction from well P3, was mutagenic without S9

Table 16. The mutagenicity of aromatic hydrocarbon fractions and subfractions of heavy oils, heavy oil products, and recovered oils as determined by the Ames _Salmonella_/microsome assay.

Sampling Location and Sample Number	Sample Description	BaP Content (μg/g of oil)	Revertants per mg of fraction		Revertants per g of produced oil	
			+S9	-S9	+S9	-S9
Southern Alberta						
28-24-12	Treater oil, subfraction	0.1	920	(-)*	570	(-)
28-24-13	Treater oil, subfraction	0.0	4000	(-)	1300	(-)
28-13-6	Well P3 oil, subfraction	3.5	740	(-)	560	(-)
28-13-7	Well P3 oil, subfraction	0.7	650	140	490	70
28-5-9	Well P1 oil, subfraction	1.4	2100	(-)	600	(-)
28-9-9	Well P2 oil, subfraction	0.7	1500	(-)	670	(-)
28-17-9	Well P4 oil, subfraction	0.3	1400	(-)	570	(-)
UMATAC Process						
25-3-2	Day tank oil, fraction	ND	(-)	57	(-)	6100
25-27-11	Overhead oil, subfraction	ND	2700	(-)	1700	(-)
25-27-13	Overhead oil, subfraction	ND	6000	(-)	300	(-)
Combustion Tube						
35-2-2	Produced oil, basic fraction	ND	(-)	(-)	(-)	(-)
35-2-3	Produced oil, acid fraction	ND	(-)	(-)	(-)	(-)
35-4-10	Produced oil, subfraction	1.9	1850	(-)	180	(-)
35-4-12	Produced oil, subfraction	0.2	740	(-)	190	(-)
Peace River						
99-24-5	Well 44 oil, subfraction	ND	30	130	90	440
99-24-16	Well 44 oil, subfraction	1.7	2509	400	7500	1200
99-24-30	Well 44 oil, subfraction	ND	2200	890	280	46
99-26-21	Top oil, subfraction	ND	(-)	(-)	(-)	(-)
99-28-25	Vacuum gas oil, subfraction	ND	3500	1400	340	130
99-30-5	Pitch, subfraction	ND	90	26	100	29
99-30-11	Pitch, subfraction	ND	290	240	96	79
99-30-21	Pitch, subfraction	ND	3900	(-)	380	(-)
99-30-41	Pitch, subfraction	ND	1800	1500	29	82
99-30-71	Pitch, subfraction	ND	9400	880	160	15
99-30-72	Pitch, subfraction	ND	1400	460	65	21
Brooks						
11-30-5	Recovered oil, fraction	ND	260	130	51000	25000
Grande Prairie						
11-34-5	Recovered oil, fraction	ND	(-)	(-)	(-)	(-)

* (-) no detectable mutagenic activity
ND = not determined

activation and the activity was relatively low at 70 revertants per gram of oil. There was no direct relationship between benzo(a)pyrene content and mutagenic activity. The aromatic subfraction which produced the greatest number of revertants contained no detectable benzo(a)pyrene. It did, however, contain compounds of mass 228, 242, 256, and 270, indicative of alkylated benzanthracenes, chrysenes, and triphenylenes, some of which are known or suspected to be mutagenic. The lack of a correlation between benzo(a)- pyrene and mutagenicity in the Ames test would be partly caused by varying degrees of suppression of activity by differing hydrocarbon matrices. The lack of benzo(a)-pyrene in the most mutagenic fraction from the SHOP project illustrates that benzo(a)pyrene alone is not a good indicator of the biological activity of a produced oil.

3.3.3.2 UMATAC Process Oils. Aromatic hydrocarbons were separated from a UMATAC day tank oil by dimethyl formamide extraction and column chromatography. Twenty-seven percent of the original oil was extractable with DMF and column chromatography of which 63%, or 17% of the original oil, was aromatic hydrocarbons.

The benzo(a)pyrene content of the sample was 16 µg/g oil, a relatively high value as compared with that of normal crude oils and some heavy oils. The total aromatic hydrocarbon fraction, without further separation, was tested for biological activity with the Ames test. No activity was found in the presence of the S9 microsomal enzymes (Table 16). This is understandable in view of the suppression of the activity of mutagens in the Ames test when large amounts of non-mutagenic hydrocarbons are present. The aromatic fraction showed mutagenic activity in the absence of S9 - 56 revertants per mg of aromatic material or 6100 revertants per gram of whole oil. This activity is due to direct acting mutagens rather than the polycyclic aromatic hydrocarbons which would require microsomal enzymes to convert them into active compounds.

The overhead oil was similarly extracted with DMF and the aromatic hydrocarbons separated by column chromatography. The aromatic hydrocarbons were then further separated into subfractions on a second alumina column. The benzo(a)pyrene content of the overhead oil was low being only 2.9 µg/g. Two of the subfractions, when tested for mutagenicity, showed mutagenic activity in the presence of S9: 2700 and 6000 revertants per mg of aromatic material or 1700 and 300 revertants per mg of the original oil. No activity was found in the absence of S9. The finding of mutagenic activity in these two fractions was expected because they contained benzo(a)pyrene and numerous other compounds which are likely to be mutagenic or carcinogenic. The mutagenicity was not great when compared with that of the refinery residuals as shown in Table 17.

3.3.3.3 Peace River In-situ Project. Oil and water produced as an emulsion from the AOSTRA-Shell Peace River project, well 44, contained 2.7 µg/g benzo(a)pyrene. Since this emulsion was about 65% water, the benzo(a)pyrene content of the oil alone was 7.7 µg/g. Aromatic subfractions from the oil showed mutagenic activity both in the presence and absence of S9, indicating that both direct acting mutagens, and mutagens which required enzyme activation, were present. Although the mutagenicity of one aromatic subfraction was high as compared with other heavy oils (Table 16) the activity was considerably less than that of refinery residuals (Table 17).

Vacuum gas oil from the diluent recovery unit contained 1.7 µg/g benzo(a)pyrene. In the presence of S9 an aromatic subfraction of the vacuum gas oil gave a mutagenicity of 3500 revertants per mg or 340 revertants per gram of original oil. Surprisingly, the pitch from the diluent recovery unit contained only 1.9 µg/g benzo(a)pyrene. Aromatic subfractions of the pitch gave up to 9400 revertants per mg in the Ames test but the mutagenicity per g of pitch was low as compared with that of refinery residuals. Top oil contained only 0.1 µg/g benzo(a)pyrene and showed no mutagenic activity.

3.3.3.4 Combustion Tube Experiments. A single sample of heavy oil (159-11) from the University of Calgary combustion tube experiments was examined. The benzo(a)pyrene content of the oil, 2.6 µg/g, was similar to that of other heavy oils produced from the Athabasca oil sands but not as high as that found in the Gregoire Lake in-situ

Table 17. The mutagenicity of aromatic hydrocarbon fractions and subfractions of refinery residuals from Sarnia, Ontario.

Sampling Location and Sample Number	Sample Description	BaP Content (μg/g oil)	Revertants per mg of sample		Revertants per g of sample	
			+S9	-S9	+S9	-S9
Catalytic Cracker						
25-11-8	Heavy cycle oil, subfraction		4400	(-1)	44 000	(-)
25-11-9	Heavy cycle oil, subfraction		7400	1200	29 000	4800
25-11-11	Heavy cycle oil, subfraction	38	2900	(-)	6100	(-)
25-11-13	Heavy cycle oil, subfraction	9.1	15 000	470	40 000	1100
25-11-14	Heavy cycle oil, subfraction	1.4	16 000	450	19 000	540
25-11-15	Heavy cycle oil, subfraction		15 000	(-)	40 000	(-)
25-5-2	Fractionator bottoms, fraction	1050	(-)	609	(-)	250 000
25-6-8	Fractionator bottoms, subfraction		5700	470	5400	450
25-6-25	Fractionator bottoms, subfraction		2800	470	1400	240
25-6-28	Fractionator bottoms, subfraction		6200	370	4700	280
Steam Cracker						
25-7-9	Tar, subfraction		4500	320	26 000	1900
25-7-10	Tar, subfraction		5400	310	18 000	1000
25-7-11	Tar, subfraction		6400	230	12 000	430
25-7-17	Tar, subfraction		5600	(-)	1500	(-)
25-7-20	Tar, subfraction		8000	500	1500	90
Fluid Coker						
25-15-13	Heavy gas oil, subfraction	4.7	8300	970	8200	970
25-15-14	Heavy gas oil, subfraction	0.7	32 000	300	19 000	180
25-15-15	Heavy gas oil, subfraction		2200	(-)	1300	(-)

combustion products. Aromatic hydrocarbon subfractions of the combustion tube oil showed mutagenicity in the same range as other heavy oils, 1850 and 740 revertants per mg of sample or 180 and 190 revertants per gram of oil, with S9 enzyme activation. No mutagenic activity was found in the absence of S9.

Organic bases were extracted from the combustion tube oil with hydrochloric acid and acidic organic compounds with sodium hydroxide. Neither the organic acids nor the bases showed mutagenicity with or without S9 enzymes.

3.3.3.5 Refinery Residuals. Catalytic cracker fractionator bottoms obtained from a refinery at Sarnia, Ontario were fractionated and the aromatic fraction was analysed for benzo(a)pyrene by gas chromatography-mass spectrometry. The BaP content was high at 1050 µg per gram of bottoms. Despite the high BaP content, the mutagenic activity of the whole aromatic fraction was low, 12 revertants per mg or 660 revertants per gram on a whole oil basis (Table 17). As discussed previously, mutagenic activity in the Ames test is suppressed by the presence of non-mutagenic hydrocarbons in the aromatic fraction. The aromatic fraction did show activity when tested on strain TA98 in the absence of the S9 enzymes, indicating the presence of direct acting mutagens. The activity under these conditions was 610 revertants per mg of aromatics or 33 400 revertants per g of oil. The high benzo(a)pyrene content and relatively high mutagenic activity in the absence of S9 indicates that these refinery bottoms are likely to have far greater biological activity than any of the in-situ combustion products or heavy oils recovered by in-situ methods.

Steam cracker refinery tar also contained relatively large amounts of benzo(a)pyrene, 150 µg per gram of tar, or 220 µg per gram of the maltene fraction of the tar. A large percentage, 55%, of the maltene fraction was soluble in DMF and, upon column chromatography on alumina, 90% of this was found to be aromatic hydrocarbons. These aromatic hydrocarbons were further fractionated into groups of compounds by chromatography on a second alumina column. Each subfraction was then analysed by combined gas chromatography-mass spectrometry and the mutagenicity determined by the Ames test. The total benzo(a)pyrene content of the sample was over 150 μg/g oil and some aromatic subfractions contained as much as 280 μg of BaP. Not surprisingly, all the subfractions showed mutagenic activity, up to 8000 revertants per mg. The activity was less, however, than would be produced by a similar amount of benzo(a)pyrene alone, again illustrating the suppression of mutagenicity by non-mutagens in the Ames test.

The catalytic cracker heavy cycle oil contained even larger amounts of benzo(a)pyrene, 240 μg/g oil, and showed the highest mutagenic activity of any of the oils tested. The activity of aromatic hydrocarbon subfractions of the oil ranged from 2900 to 16 000 revertants per mg, up to 44 000 revertants per gram of oil. The fluid coker heavy gas oil also contained substantial amounts of benzo(a)pyrene, 91 μg/g, and displayed high mutagenic activity. One aromatic hydrocarbon subfraction gave 32 000 revertants per mg and 19 000 revertants per g of oil. In the case of both oils, most of the mutagenic activity occurred in the presence of S9 enzymes and was likely caused by polycyclic aromatic hydrocarbons. Some mutagenicity in the absence of S9 was observed, thus indicating the presence of other types of mutagens.

3.3.4 Microtox Toxicity Testing of Produced Waters.

3.3.4.1 Gregoire Lake Pilot. The Microtox system was used to test the toxicity to aquatic organisms of produced waters (1) as received, (2) after purging with helium to remove volatile organic components, and (3) after extraction to remove acidic, basic, and neutral compounds.

All samples from the Gregoire Lake Pilot project were toxic as received with EC_{50} values ranging from 0.30 to 11.4 (Table 18). Low EC_{50} values indicate the presence of significant amounts of toxic compounds whereas values over 80 indicate little or no toxic material. Among the most toxic samples were the COFCAW-produced waters, GP26 sampled in March and May, and the fluids produced by steam stimulation from well GP31. The fluids from GP31 contained large amounts of dispersed clay minerals and bitumen with a total organic carbon content of 1850 ppm. In both cases, the waters were found to be highly toxic to

Table 18. The toxicity of Gregoire Lake pilot waters as determined with the Microtox system.

	As Received		Volatile Free		Extracted		Double Extracted	
Sample	$EC_{50}(5)^{a}$	$EC_{50}(15)^{b}$	$EC_{50}(5)$	$EC_{50}(15)$	$EC_{50}(5)$	$EC_{50}(15)$	$EC_{50}(5)$	$EC_{50}(15)$
<u>Gregoire Lake</u>								
GP-20 (Feb)	7.2	11.5	21	18	323	77		
GP-20 (Mar)	11.4	11.0	57	49	NE	NE		
GP-21 (Feb)	2.2	2.9	16	14	88	153		
GP-21 (Mar)	2.6	2.9	12	8.9	37	36		
GP-21 (Jun)	1.1	1.3	4.6	4.4	80	121		
GP-26 (Feb)	2.5	3.2	4.6	5.0	26	27	135	153
GP-26 (Mar)	.84	.96	2.0	2.2	22	18		
GP-26 (May)	.61	.74	-	-	17	16	81	81
GP-26 (Jun)	2.2	2.2	2.8	3.0	-	-		
GP-31 (Feb)	.30	.32	.39	.58	33	35		
GP-31 (Mar)	.31	.41	.54	1.4	36	36		
GP-19 (May)	2.8	3.0	17	16	61	64		
GP-19 (Jun)	1.3	1.5	11	11	93	126		
Peace River Well No. 44	0.98	1.11	0.52	0.59				

[a] (5) - 5 minute values
[b] (15) - 15 minutes values
NE = no significant effect

aquatic organisms. EC_{50} values measured after 15 minutes did not vary greatly from those measured after 5 minutes.

Purging with helium to remove volatile organic compounds reduced, but did not remove, the toxicity of the produced waters.

Among the major groups of compounds removed from the samples by purging were benzene and alkyl substituted benzenes. The toxicity of these compounds to aquatic organisms is well known; therefore, their removal from the samples should have reduced the toxicity. However, the samples after purging were still toxic with values ranging from 0.39 to 57. Samples GP26 and GP31 were still highly toxic.

Extraction of the produced waters with toluene, a total of nine times at three different pH conditions, greatly reduced the toxicity of all samples. Five of the 13 samples showed little or no toxicity after extraction. Thus, the extractable organic material in the produced waters, rather than the volatile organic compounds or inorganic constituents, was responsible for the majority of the observed toxicity.

A major group of organic compounds extracted from the waters were phenolics: phenol, alkyl substituted phenols, and alkyl substituted napthalenol. The COFCAW-produced water contained 0.62 µg/mL methylphenols, 1.2 µg/mL dimethylphenols, and 0.38 µg/mL trimethyl phenols. As no special precautions were used to preserve the samples, some losses of phenols likely occurred and these concentrations are probably low. These compounds are highly toxic to aquatic organisms. Also found were many alkyl substituted benzoic acids, substituted aromatic hydrocarbons, benzenamines, pyridines, and quinolines. These compounds would readily account for the observed toxicity of the extractable organic materials from the produced waters.

Despite repeated extractions under acid, basic, and neutral conditions, a strong odour of phenols was apparent in some of the extracted samples. Apparently not all the phenols were totally extracted from the sample. Consequently, three samples were further extracted under acid conditions. These doubly extracted samples were then tested for toxicity. In all cases, they were non-toxic, confirming that the major cause of toxicity in the produced waters was the extractable organic compounds.

Table 19. The toxicity of produced waters as determined with the Microtox system.

	Original		Volatile Free		After Extraction	
Sample	$EC_{50}(5)$	$EC_{50}(15)$	$EC_{50}(5)$	$EC_{50}(15)$	$EC_{50}(5)$	$EC_{50}(15)$
Treater water Southern Alberta, 1983 January	0.54	0.69	1.3	1.5	54	46
Treater water Southern Alberta, 1983 May	0.49	0.38	0.78	0.70	40	42
Peace River Well 44 water	0.98	1.11	0.52	0.59	78	63
UMATAC overhead vent water	0.12	0.12	0.27	0.30	4.0	4.7
UMATAC preheat vent condensed water	1.12	0.61	1.44	0.94	28	23
UMATAC scrubber settling tank underflow	9.8	9.3	10	12	57	82

(5) - 5 minute values
(15) - 15 minute values

3.3.4.2 SHOP Project. Two water samples from the Southern Alberta in-situ combustion project were biologically tested and chemically analysed by combined gas chromatography-mass spectrometry. Treater water collected in January had a pH of 8.2, a total organic carbon content of 204 ppm, and a volatile carbon content of 30 ppm. A similar sample collected in May contained 511 ppm total organic carbon and 171 ppm volatile organic carbon. Both showed toxicity to aquatic organisms by the Microtox test (Table 19). Five minute EC_{50} values were 0.54 and 0.49 indicating a high toxicity. Removal of the volatile components reduced the toxicity by about 50% but the volatile free samples were still highly toxic. Extraction of the organic compounds greatly reduced the toxicity and the organic free samples were only slightly toxic. These results indicate that organic, rather than inorganic compounds, were responsible for the toxicity. The volatile components were purged from the water samples and analysed by gas chromatography-mass spectrometry. A multitude of organic compounds was detected. Major components were alkyl substituted cyclohexanes and cyclopentanes. Also present were benzene, toluene, xylenes, trimethylbenzenes, naphthalene, dimethyl naphthalenes, and trimethyl naphthalenes. These aromatic hydrocarbons are toxic to fish and would account for the toxicity of the volatile components of the treater waters.

3.3.4.3 UMATAC Process. Three water samples from the UMATAC project were examined. The pH of the samples was low, ranging from 2.5 to 4.4. The organic carbon content of the overhead vent water was high, 4890 ppm, of which 90 ppm was volatile material. The other two water samples, the preheat vent condensed water and the scrubber settling tank underflow water, contained 634 ppm and 68 ppm organic carbon, respectively. The volatile organic carbon content of these samples was less than 3 ppm.

Prior to testing for toxicity with the Microtox bioluminescence system, the pH of the samples was adjusted to near seven with sodium hydroxide. The overhead vent water and the preheat vent condensated water were both highly toxic with EC_{50} five minute values of 0.12 and 1.12 (Table 19). The overhead vent water showed the most toxicity of any of the produced or waste waters tested with the Microtox system. The scrubber settling tank water was somewhat less toxic with a five minute EC_{50} value of 9.8. Some of the toxicity was due to volatile organic compounds but the majority was caused by extractable organic compounds. The overhead vent water was still highly toxic after extraction of the organic compounds. This toxicity may be caused by inorganic compounds or incomplete extraction of the large amount of organic materials originally present.

3.3.4.4 Peace River Pilot Project. Water separated from the oil-water emulsion produced by well 44 of the Peace River Pilot project had a pH of 6.4 and an organic carbon content of 376 ppm of which 59 ppm was volatile organic carbon. As was the case with other waters co-produced with heavy oil from in-situ recovery processes, the water from well 44 was highly toxic in the Microtox bioluminescence assay (Table 19) as indicated by the five minute EC_{50} value of 1.0. Purging with helium did little to alter the toxicity of the sample, indicating that volatile organic compounds were not a major contributor to toxicity.

In the event that produced hydrocarbons were to come in contact with surface waters, it might be expected that some toxicity would be imparted to the waters. Water was contacted with various amounts of top oil, vacuum gas oil, and diluent from the Peace River process. EC_{50} five minute values ranged from 0.4 when 50 mL of diluent was in contact with 1 litre of water for 24 hours, to 31 when 0.5 mL of vacuum gas oil was contacted with 1 litre of water (Table 20). The toxicity roughly followed the concentration of organic carbon in the contaminated water. The most toxic sample which had been in contact with diluent contained 97 µg/g total organic carbon, whereas the least toxic contained 4 µg/g total organic carbon. Purging the water with air, after removal of the liquid hydrocarbon phase, reduced the toxicity of the waters by about 25%.

3.3.4.5 Combustion Tube Experiments. A series of 10 water samples from a "wet" combustion tube experiment were analysed for total organic carbon and volatile organic carbon, and were tested for toxicity using

Table 20. Toxicity of waters after contact with oils as determined by the Microtox test.

						Volatile Free	
Sample	mL oil per L water	TOC (ppm)	VOC (ppm)	$EC_{50}(5)$	$EC_{50}(15)$	$EC_{50}(5)$	$EC_{50}(15)$
<u>Peace River</u>							
Vacuum gas oil	0.5	3.55	0.99	31.3	29.3	28.8	25.3
	1.0	4.60	0.53	10.9	10.1	15.1	13.4
	5.0	6.17	1.13	10.3	10.0	13.3	13.3
	10.0	8.32	1.68	6.2	5.6	5.8	4.3
	50.0	22.66	1.04	2.2	2.5	2.8	13.3
Top Oil	0.5	9.47	7.14	9.7	12.5	33.9	42.3
	1.0	20.33	13.76	8.6	9.4	17.9	21.9
	5.0	45.77	22.46	2.4	2.8	4.8	5.7
	10.0	59.81	14.56	1.7	1.7	2.9	3.5
	50.0	158.2	15.20	0.64	0.69	0.66	0.69
Diluent	0.5	6.36	2.15	7.1	6.9	8.8	8.8
	1.0	9.88	2.93	4.1	3.9	5.7	5.5
	5.0	31.68	6.91	1.8	1.8	2.2	2.3
	10.0	45.44	5.18	1.0	0.92	0.95	0.86
	50.0	97.46	7.82	0.37	0.37	0.41	0.39

the Microtox system (Table 21). The total organic carbon content (TOC) of the 10 samples ranged from 1030 to 6390 ppm with the waters produced earlier in the experiment having the lowest total organic carbon content. Volatile organic carbon (VOC) ranged from 40 to 350 ppm with waters produced later in the experiment having the highest volatile organic carbon and the lowest pH, 1.6. $EC_{50}(5)$ and $EC_{15}(15)$ values were lowest, indicating the highest toxicity, for samples with high total organic carbon and low pH. (The pH was adjusted to 7 prior to toxicity testing.) The lowest EC_{50} value of 0.42 was in the same range as waters produced from the Gregoire Lake and SHOP pilot projects. These waters were far less toxic than UMATAC overhead vent waters but nevertheless showed a high toxicity to aquatic organisms.

Table 21. The acidity, organic carbon content, and toxicity of combustion tube waters as determined with the Microtox system.

Sample	pH	Volatile Organic Carbon (ppm)	Total Organic Carbon (ppm)	As Received		Volatile Free	
				$EC_{50}(5)$[a]	$EC_{50}(15)$[b]	$EC_{50}(5)$	$EC_{50}(15)$
168-9	7.5*	55	1034	0.82	0.73	1.52	1.59
168-12	7.5*	112	1200	0.65	0.58	1.15	1.00
168-6	5.2	60.6	1308	4.6	4.2	6.3	4.1
169-8	4.0	41	1313	5.7	4.5	7.5	6.5
169-9	4.1	100	1570	9.7	9.4	13.3	12.0
169-11	2.6	296	4811	1.7	1.2	1.5	1.2
169-13	2.2	180	4057	1.7	1.2	2.0	1.3
169-15	1.6	47	6389	0.78	0.38	1.6	0.82
169-18	1.7	353	5566	0.57	0.42	0.74	0.56
169-20	1.7	227	4137	0.75	0.46	0.94	0.89

[a] (5) - 5 minutes values

[b] (15) - 15 minutes values

* pH determined using indication sticks.

All samples were shaken filtered, and pH adjusted to 7 before toxicity determinations.

Carbon content was determined on a settled filtered sample.

pH readings were taken using a micro-electrode.

4. SUMMARY AND CONCLUSIONS

The objective of this project was to assess possible environmental hazards and human health risks arising from toxic and carcinogenic materials during recovery of heavy oil by in-situ methods. The more specific objectives were: (1) to chemically identify hazardous constituents of produced fluids; (2) to biologically test their toxicity and mutagenicity; (3) to relate their formation to production conditions; and, (4) to evaluate possible hazards in comparison with those of conventional and other synthetic fuels.

It should be noted that present methods of chemical analysis and short-term biological tests, such as applied in this study, are at best only indicators of potential human health risks or environmental hazards. They are not definitive, but do allow comparisons to be made of chemical composition and biological properties of oils and waters from conventional production and synthetic oil processes.

The results of the study are as follows:

1. Chemical analysis revealed the presence of known carcinogens and mutagens in oils produced by in-situ combustion from Gregoire Lake and from Suffield pilot projects. Unaltered Athabasca bitumen, unaltered Suffield heavy oil, commercially produced "synthetic" crude oil from the Athabasca oil sands, conventional crude oils, and heavy oil produced by steam injection from the Athabasca and Peace river oil sands, and from Suffield, all contained benzo(a)pyrene and other known carcinogens and mutagens.

2. The concentrations of benzo(a)pyrene in the oils produced by in-situ combustion and steam injection were in the same concentration range as those of conventional crude oils and heavy oils, 1 to 20 ppm, and far less than those found in refinery residuals, 90 to 1050 ppm, or reported in some fuel oils and coal tars, up to 10 000 ppm.

3. Oils from the UMATAC dry retorting process contained higher concentrations of benzo(a)pyrene, up to 32 ppm, than found in oils produced by in-situ combustion or steam injection, 0.9 to 14 ppm. Furthermore, the oils from the dry retorting process contained relatively high concentrations of nitrogen containing aromatic compounds, some of which are known or suspected to be carcinogenic or mutagenic.

4. The mutagenicity of oils produced by in-situ combustion, as indicated by the Ames test conducted on chemically separated fractions of the oils, was similar to that of oils produced by steam injection and well below the activity of refinery bottoms, tars, and pitches.

5. Waters co-produced with oil from in-situ recovery pilot plants contained many low molecular weight aromatic compounds, phenols, and nitrogen compounds in concentrations toxic to aquatic organisms.

6. Waters produced from the Gregoire Lake Pilot Study, the Suffield Heavy Oil Project, and the Peace River Project were all toxic to aquatic organisms in the Microtox system. Waters were judged to be "strongly" toxic, requiring dilutions of 10 to 300 times, to bring them into the non-toxic range. Some of the toxicity was caused by volatile organic compounds but the majority was caused by extractable organic compounds, primarily alkylated phenols and naphthalenes.

7. Waters from the UMATAC dry retorting process contained high concentrations of nitrogen compounds such as pyridines, pyrimidines, aminoindans, and quinolines. These waters were three times more toxic than any water from in-situ combustion pilot projects tested during this study.

The chemical analyses and limited biological testing carried out in this study detected no potential for a strong carcinogenic hazard associated with in-situ recovery of heavy oil by combustion and steam injection methods. The relative hazard is probably marginally greater than that associated with production of conventional light crude oils but far less than might be expected from coal liquefaction processes or from the disposal of refinery residuals. The hazard associated with dry retorting is greater than that from in-situ recovery methods and care should be taken in the handling of both products and wastewaters from this process.

The presence of many low molecular weight aromatic hydrocarbons, nitrogen compounds, and phenols in waters from in-situ pilot plants and the dry retorting process is of environmental concern. Not only are these compounds toxic in low concentrations to aquatic organisms, but they impart taste and odour to drinking water. Should waters from the combustion zone contaminate groundwater aquifers or surface waters, dilutions of 10 to 900 times would be required to reduce toxicity to aquatic organisms and dilutions of 3000 times or more would be required to reduce taste and odour effects.

5. REFERENCES

Adamek, E.G. 1972. An efficient separation of B(a)P from B(k)F and their fluorescence determination in air samples. ACS National Conference. New York. 14 pp.

Adams, E.A., E.J. Lavoie, and D. Hoffmann. 1983. Mutagenicity and metabolism of Azaphenanthrenes. In: M. Cooke and A.J. Dennis, eds. Polynuclear Aromatic Hydrocarbons: Formation, Metabolism and Measurement. Columbus, Ohio:Battelle Press. pp. 73-84.

Ames, B.N., J. McCann, and E. Yamasaki. 1975. Methods for detecting carcinogens and mutagens with the Salmonella/mammalian-microsome mutagenicity test. Mutation Research 31: 347-364.

Anderson, J.W., J.M. Negg, B.A. Cox, H.E. Tatem, and G.M. Hightower. 1974. Characteristics of dispersions and water-soluble extracts of crude and refined oils and their toxicity to estuarine Crustaceans and fish. Marine Biology 27: 75-88.

Ball, L.M., M.J. Kohan, L.D. Claxton, and J. Lewtas. 1984. Mutagenicity of derivatives and metabolites of 1-nitropyrene: activation by rat liver S9 and bacterial enzymes. Mutation Research 138: 113-125.

Bingham, E. and W. Barkley. 1979. Bioassay of complex mixtures derived from fossil fuels. Environmental Health Perspectives 30: 157-163.

Bridge, J.C. and S.A. Henry. 1928. Industrial cancers. In: Report of the International Conference on Cancer. 1928 July 17-20. London. New York:William Wood and Company. pp. 258-268.

Brown, J.M., S.A. Wise, and W.E. May. 1980. Determination of Benzo(a)-pyrene in recycled oils by a sequential HPLC method. Journal of Environmental Science and Health A15(6): 613-623.

Bulich, A.A., M.W. Greene, and D.L. Isenberg. 1980. The reliability of the bacterial luminescence assay for the determination of toxicity of pure compounds and complex effluents. Aquatic Toxicity and Hazard Assessment: Fourth Conference, ASTM STP 737, D.R. Branson and K.L. Dickson, eds. American Society for Testing and Materials, pp. 338-347.

Chang, J.C., P.B. Taylor, and F.R. Leach. 1981. Use of the Microtox assay system for environmental samples. Bulletin of Environmental Contamination and Toxicology 26: 150-156.

Colmsjö, A., A. Rannug, and U. Rannug. 1984. Some chloro derivatives of polynuclear aromatic hydrocarbons are potent mutagens in Salmonella typhimurium. Mutation Research 135: 21-29.

Coombes, R.M. and K.A. Hazer. 1982. Comparison of the carcinogenic potential of crude oil and shale oil. In: H.N. MacFarland, C.E. Holdsworth, J.A. MacGregor, R.W. Call, and M.L. Kane, eds. The Toxicology of Petroleum Hydrocarbons, Symposium Proceedings. American Petroleum Institute. 1982 May, Washington, D.C. pp. 208-224.

Coombs, M.M., C. Dixon, and A. Kissonerghis. 1976. Evaluation of the mutagenicity of compounds of known carcinogenicity, belonging to the benz(a)anthracene, chrysene, and cyclopenta(a)phenanthrene series, using Ames's test. Cancer Research 36: 4525-4529.

Coomes, R.M. 1976. Health effects of oil shale processing. Quarterly of the Colorado School of Mines 71(4): 101-123.

DeFlora, S., P. Zanacchi, A. Camoirano, C. Bennicelli, and G.S. Badolati. 1984. Genotoxic activity and potency of 135 compounds in the Ames reversion test and in a bacterial DNA-repair test. Mutation Research 133: 161-198.

Dickson, K.L. 1982. Research needs in aquatic toxicology and hazard assessment: a sojorner's perspective. Proceedings of the Fifth Annual Symposium on Aquatic Toxicology, American Society for Testing Materials. 1980 October 7-8; Philadelphia, Pennsylvania; ASTMP766: 9-14.

Dipple, A. 1976. Polynuclear aromatic carcinogens. In: C.E. Searle, ed. Chemical Carinogens, ACS Monograph 173. Washington, D.C.: American Chemical Society. pp. 245-314.

Durand, J.P. and N. Petroff. 1979. Determination of benzo(a)pyrene and other polyaromatic hydrocarbons in petroleum oils by direct liquid chromatography. Chromatographia 12,497: 85-95.

Epler, J.L., J.A. Young, A.A. Hardigree, T.K. Rao, M.R. Guerin, I.B. Rubin, C.-H. Ho, and B.R. Clark. 1978. Analytical and biological analyses of test materials from the synthetic fuel technologies. I. Mutagenicity of crude oils determined by the Salmonella typhimurium/Microsomal Activation System. Mutation Research 57: 265-276.

Epler, J.L., F.W. Larimer, T.K. Rao, C.E. Nix, and T. Ho. 1978. Energy-related pollutants in the environment: use of short-term tests for mutagenicity in the isolation and identification of biohazards. Environmental Health Perspectives 27: 11-20.

Epler, J.L., T.K. Tao, and M.R. Guerin. 1979. Evaluation of feasibility of mutagenic testing of shale oil products and effluents. Environmental Health Perspectives 30: 179-184.

Freudenthal, R.I., G.A. Lutz, and R.I. Mitchell. 1975. Carcinogenic potential of coal and coal conversion products. Columbus, Ohio:Battelle Columbus Laboratories.

Guerin, M.R. 1977. Energy sources of polycyclic aromatic hydrocarbons. Oak Ridge, Tennessee:Oak Ridge National Laboratory. 78 pp.

Guerin, M.R., C.-H. Ho, T.K. Rao, B.R. Clark, and J.L. Epler. 1980. Polycyclic aromatic primary amines as determinant chemical mutagens in petroleum substitutes. Environmental Research 23: 42-53.

Grimmer, G. and A. Hildebrandt. 1972. Concentration and estimation of 14 polycyclic aromatic hydrocarbons at low levels in high protein foods, oils and fats. Journal of Associated Official Analytical Chemistry 55: 631.

Haagensen, C.D. 1931. Occupational neoplastic disease. American Journal of Cancer 15: 641-703.

Harrison, W., M.A. Winnik, P.T.Y. Kwong, and D. Mackay. 1975. Disappearance of aromatic and aliphatic components from small sea-surface slicks. Environmental Sciences and Technology 9(3): 231-234.

Heller, I. 1930. Occupational cancers. Journal of Medical Hygiene 12: 169-197.

Helmes, C.T., D.L. Atkinson, J. Jaffer, C.C. Sigman, and K.L. Thompson. 1982. Evaluation and classification of the potential carcinogenicity of organic air pollutants. Journal of Environmental Science and Health A17(3): 321-389.

Henry, S.A. 1947. Occupational cutaneous cancer attributable to certain chemicals in industry. British Medical Bulletin 4: 389-401.

Holland, L.M. and C.G. Stafford. 1981. The Los Alamos integrated oil shale health and environmental program: A status report. LA-8665-SR. Los Alamos, New Mexico:Los Alamos Scientific Laboratory, University of California.

Jewell, D.M., J.H. Weber, J.W. Bunger, H. Plancher, and D.R. Latham. 1972. Ion-exchange, coordination, and adsorption chromatographic separation of heavy-end petroleum distillates. Analytical Chemistry 44: 1391-1395.

Kaden, D.A., R.A. Hites, and W.G. Thilly. 1979. Mutagenicity of soot and associated polycyclic aromatic hydrocarbons to Salmonella typhimurium. Cancer Research 39: 4152-4159.

Kimball, R.F. and N.B. Munro. 1981. A critical review of the mutagenic and other genotoxic effects of coal liquefaction. Report OPNL-5721. Oak Ridge, Tennessee:Oak Ridge National Laboratory. pp. 199.

Klopman, G. and H.S. Rosenkranz. 1984. Structural requirements for the mutagenicity of environmental nitroarenes. Mutation Research 126: 227-238.

Kornreich, M.R. 1976. Coal conversion processes: potential carcinogenic risk. MTR-7155, Baileys Crossroads, VA: Mitre Corporation. Technical Report. pp. 4-14 to 4-16.

Ladner, A. 1982. 4-Chloromethylbiphenyl (4CMB), benzyl chrloride (BC) and 4-hydroxymethylbiphenyl (4HMB): Reverse mutation tests with Salmonella typhimurium. Mutation Research 100: 27-31.

Later, D.W., R.A. Pelroy, D.D. Mahlum, C.W. Wright, M.L. Lee, W.C. Weimer, and B.W. Wilson. 1983. Identification and comparative genotoxicity of polycyclic aromatic hydrocarbons and related nitrogen-containing heteratomic species in products from coal liquefaction processes. In: M. Cooke and A.J. Dennis, eds. Polynuclear Aromatic Hydrocarbons: Formation, Metabolism and Measurement. Columbus, Ohio: Battelle Press. pp. 771-783.

LaVoie, E., L. Tulley, V. Bedenko, and D. Hoffmann. 1979. Mutagenicity, tumor initiating activity, and metabolism of tricyclic polynuclear aromatic hydrocarbons. In: A. Bjorseth and A.J. Dennis, eds. Polynuclear Aromatic Hydrocarbons: Chemistry and Biological Effects. Columbus, Ohio: Battelle Press. pp. 1041-1057.

LaVoie, E.J., L. Tulley-Freiler, V. Bedenko, Z. Girach, and D. Hoffman. 1981. Comparative studies on the tumor initiating activity and metabolism of methylfluorenes and methylbenzofluorenes. In: M. Cooke and A.J. Dennis, eds. Polynuclear Aromatic Hydrocarbons: Chemical Analyses and Biological Fate. Columbus, Ohio:Battelle Press. pp. 417-427,

LaVoie, E.J., G. Briggs, V. Bedenko, and D. Hoffmann. 1982. Mutagenicity of substituted carbazoles in Salmonella typhimurium. Mutation Research 101: 141-150.

LaVoie, E.J., L. Tulley-Freiler, V. Bedenko, and D. Hoffmann. 1983. Mutagenicity of substituted phenanthrenes in Salmonella typhimurium. Mutation Research 116: 91-102.

LaVoie, E.J., D.T. Coleman, R.L. Tonne, and D. Hoffman. 1983. Mutagenicity, tumor initiating activity and metabolism of methylated anthracenes. In: M. Cooke and A.J. Dennis (eds.) Polynuclear Aromatic Hydrocarbons: Formation, Metabolism and Measurement. Columbus, Ohio: Battelle Press. pp. 785-798.

Lebsack, M.E., A.D. Anderson, G.M. DeGraeve, and H.L. Bergman. 1981. Comparison of bacterial luminescence and fish bioassay results for fossil-fuel process waters and phenolic compounds. Proceedings of the Fourth Annual Symposium on Aquatic Toxicology, American Society for Testing Materials. 1979; Chicago, Illinois; pp. 348-256.

Lee, M.L. and R.N. Castle. 1980. Identification of sulfur heterocycles in coal liquids and shale oils. Report DOE/EV/10237-2, U.S. Department of Energy, Office of Health and Environmental Research.

Levin, W., A.W. Wood, R.L. Chang, S. Kumar, H. Yagi, D.M. Jerina, R.E. Lehr, and A.H. Conney. 1983. Tumor-initiating activity of benz(c)acridine and twelve of its derivatives on mouse skin. Cancer Research 43: 4625-4628.

Mackay, D. and W.Y. Shiu. 1977. Aqueous solubility of polynuclear aromatic hydrocarbons. Journal of Chemical and Engineering Data 22(4): 399-402.

McCann, J., E. Choi, E. Yamasaki, and B.N. Ames. 1975. Detection of carcinogens and mutagens in the Salmonella/microsome test: Assay of 300 chemicals. Proceedings of National Academy of Science U.S.A. 72(12): 5135-5139.

McFall, T., G.M. Booth, M.L. Lee, Y. Tominaga, R. Pratap, M. Tedjamulia, and R.N. Castle. 1984. Mutagenic activity of methyl-substituted tri- and tetracyclic aromatic sulfur heterocycles. Mutation Research 135: 97-103.

Mossop, G.D. 1980. Geology of the Athabasca oil sands. Nature 207: 145-152.

National Academy of Science. 1972. Particulate polycyclic organic matter. Washington, D.C. 361 pp.

Neis, J.M., P.J.L. van Gemert, H.M.J. Roelofs, R.P. Bos, and P.Th. Henderson. 1984. Mutagenicity of benzidine and 4-aminobiphenyl after metabolic activation with isolated hepatocytes and liver 9000 x g supernatant from rat, hamster and guinea pig. Mutation Research 129: 13-18.

Nicholls, J.H. and R.W. Luhning. 1978. Heavy oil sand in-situ pilot plants in Alberta (past and present). In: D.A. Redford and A.G. Winestock, eds. The Oil Sands of Canada-Venezuela. Special Volume 17. Montreal: Canadian Institute of Mining and Metallurgy. pp. 527-538.

Nohmi, T., K. Yoshikawa, M. Nakadate, R. Miyata, and M. Ishidate, Jr. 1984. Mutations in Salmonella typhimurium and inactivation of Bacillus subtilis transforming DNA induced by phenylhydroxylamine derivatives. Mutation Research 136: 159-168.

Parker, K.R. 1979. PAH's in automotive lubricants. Calgary, Alberta: The University of Calgary. 165 pp. M.Sc. Thesis,

Pitts, J.N., Jr., D.M. Kokensgard, W. Harger, T.S. Fisher, V. Mejia, J.J. Schuler, G.M. Scorziell, and Y.A. Katzenstein. 1982. Mutagens in diesel exhaust particulate. Identification and direct activities of 6-nitrobenzo(a)pyrene, 9-nitroanthracene, 1-nitropyrene, and 5H-phenanthro(4,5-bcd)pyran-5-one. Mutation Research 103: 241-249.

Qureshi, A.A., K.W. Flood, S.R. Thompson, S.M. Janhurst, C.S. Inniss, and D.A. Rokosh. 1981. Comparison of a luminescent bacterial test with other bioassays for determining toxicity of pure compounds and complex effluents. Aquatic Toxicity and Hazard Assessment: Fifth Conference, ASTM STP 766. J.G. Pearson, R.B. Foster, and W.E. Bishop, eds. American Society for Testing and Materials. pp. 179-195.

Rinkus, S.J. and M.S. Legator. 1979. Chemical characterization of 465 known or suspected carcinogens and their correlation with mutagenic activity in the Salmonella typhimurium system. Cancer Research 39: 3289-3318.

Rosenkranz, H.S. 1984. Mutagenic and carcinogenic nitroarenes in diesel emissions: Risk identification. Mutation Research 140: 1-6.

Rubin, I.B., M.R. Guerin, A.A. Haridgree, and J.L. Epler. 1976. Fractionation of synthetic crude oils from coal for biological testing. Environmental Research 12: 358-365.

Schmitter, J-M., I. Ignatiadis, P. Arpino, and G. Guiochon. 1983. Selective isolation of nitrogen bases from petroleum. Analytical Chemistry 55: 1685-1688.

Schoeny, R. 1982. Mutagenicity testing of chlorinated biphenyls and chlorinated dibenzofurans. Mutation Research 101: 45-56.

Seixas, G.M., B.M. Andon, P.G. Hollingshead, and W.G. Thilly. 1982. The aza-arenes as mutagens for Salmonella typhimurium. Mutation Research 102: 201-212.

Sexton, R.J. 1960. The hazards to health in the hydrogenation of coal. Vol. IV: The control program and clinical effects. Archives of Environmental Health 1: 208-231.

Slaga, T.J., R.P. Iyer, W. Lyga, A. Secrist III, G.H. Daub, and R.G. Harvey. 1979. Comparison of the skin tumor-initiating activities of dihydrodios, diol-epoxides, and methylated derivatives of various polycyclic aromatic hydrocarbons. In: A. Bjorseth and A.J. Dennis, eds. Polynuclear Aromatic Hydrocarbons: Chemistry and Biological Effects. Columbus, Ohio:Battelle Press. pp. 753-769, Strosher, M.T. and E. Peake. 1978. Characterization of organic constitutents in waters and wastewaters of the Athabasca oil sands mining area. Prep. for Alberta Environment, Alberta Oil Sands Environmental Research Program. Report 20. Edmonton, Alberta. 71 pp.

Tikkanen, L., T. Matsushima, S. Natori, and K. Yoshirhira. 1983. Mutagenicity of natural naphthoquinones and benzoquinones in the Salmonella/microsome test. Mutation Research 124: 25-34.

Tomkins, B.A., R.R. Regan, J.E. Caton, and W.H. Griest. 1981. Liquid chromatographic determination of benzo(a)pyrene in natural, synthetic, and refined crudes. Analytical Chemistry 53: 1213-1217.

United States Environmental Protection Agency. 1977. Sampling and analysis procedures for screening of industrial effluents for priority pollutants. USEPA Effluent Guidelines Division, Washington, D.C.

Waters, M.D. 1979. A phased approach to the bioscreening of emissions and effluents from energy technologies. Proceedings of the Symposium on Potential Health and Environmental Effects of Synthetic Fossil Fuel Technologies, 1978 September 25-28. Oak Ridge, Tennessee. pp. 143-152.

6. APPENDICES

APPENDIX 6.1

Extractable constituents of SHOP treater water.

Table 6.1.1 SHOP treater water extractable aromatics, 1983 January.

Scan	M.W.	Compound	ppb
747	128	Naphthalene	9
951	148	C_5-Benzene	1
972	142	2-Methylnaphthalene	83
976	148	C_1-Benzothiophene	2
1004	148	C_1-Benzothiophene	1
1006	142	1-Methylnaphthalene	43
1148	154	Biphenyl	17
1159	162	C_2-Benzothiophene	10
1172	156	C_2-Naphthalene	18
1178	156	C_2-Naphthalene	9
1191	162	C_2-Benzothiophene	8
1192	156	C_2-Benzothiophene	119
1207	162	C_2-Benzothiophene	4
1220	156	C_2-Naphthalene	163
1223	162	C_2-Benzothiophene	10
1226	156	C_2-Naphthalene	87
1235	162	C_2-Benzothiophene	9
1256	156	C_2-Naphthalene	108
1285	156	C_2-Naphthalene	49
1292	170	C_3-Naphthalene	5
1331	176	C_3-Benzothiophene	2
1336	154	Dihydroacenaphthylene	4
1346	170	C_3-Naphthalene	11
1351	176	C_3-Benzothiophene	7
1368	176	C_3-Benzothiophene	4
1381	170	C_3-Naphthalene	45
1397	168	Dibenzofuran	27
1410	176	C_3-Benzothiophene	78
1413	170	C_3-Naphthalene	20
1429	170	C_3-Naphthalene	70
1443	176	C_3-Benzothiophene	26
1457	170	C_3-Naphthalene	115
1476	176	C_3-Benzothiophene	3
1481	184	C_4-Naphthalene	1
1515	170	C_3-Naphthalene	16
1516	166	Fluorene	26
1518	190	C_4-Benzothiophene	4
1528	170	C_3-Naphthalene	37
1544	182	C_2-Biphenyl	5
1554	190	C_4-Benzothiophene	21
1557	180	C_2-Fluorene	4
1560	182	C_2-Biphenyl	4
1570	190	C_4-Benzothiophene	8
1584	184	C_4-Naphthalene	15
1587	182	C_1-Dibenzofuran	14
1594	184	C_4-Naphthalene	11

continued...

Table 6.1.1. continued.

Scan	M.W.	Compound	ppb
1603	190	C_4-Benzothiophene	7
1609	182	C_1-Dibenzofuran	12
1605	184	C_4-Naphthalene	9
1620	190	C_4-Benzothiophene	4
1625	182	C_2-Biphenyl	5
1628	190	C_4-Benzothiophene	3
1634	204	C_5-Benzothiophene	4
1640	184	C_4-Naphthalene	20
1663	190	C_4-Benzothiophene	5
1675	184	C_4-Naphthalene	21
1678	204	C_5-Benzothiophene	3
1688	204	C_5-Benzothiophene	6
1693	190	C_4-Benzothiophene	7
1702	184	C_4-Naphthalene	27
1702	204	C_5-Benzothiophene	4
1711	204	C_5-Benzothiophene	6
1714	190	C_4-Benzothiophene	3
1717	204	C_5-Benzothiophene	3
1719	180	C_1-Fluorene	5
1728	180	C_1-Fluorene	20
1745	204	C_5-Benzothiophene	4
1746	180	C_1-Fluorene	6
1778	184	C_4-Naphthalene	12
1792	204	C_5-Benzothiophene	3
1801	184	Dibenzothiophene	60
1846	178	Phenanthrene	74
1930	194	C_2-Fluorene	8
1965	198	C_1-Dibenzothiophene	94
1997	198	C_1-Dibenzothiophene	63
2030	198	C_1-Dibenzothiophene	58
2030	192	C_1-Phenanthrene/C_1-Anthracene	25
2038	192	C_1-Phenanthrene/C_1-Anthracene	27
2067	192	C_1-Phenanthrene/C_1-Anthracene	52
2074	192	C_1-Phenanthrene/C_1-Anthracene	29
2110	212	C_2-Dibenzothiophene	13
2121	212	C_2-Dibenzothiophene	31
2144	212	C_2-Dibenzothiophene	23
2177	206	C_2-Phenanthrene/C_2-Anthracene	2
2204	206	C_2-Phenanthrene/C_2-Anthracene	12
2228	206	C_2-Phenanthrene/C_2-Anthracene	4
2253	206	C_2-Phenanthrene/C_2-Anthracene	22
2260	206	C_2-Phenanthrene/C_2-Anthracene	17
2260	226	C_3-Dibenzothiophene	12
2269	206	C_2-Phenanthrene/C_2-Anthracene	5
2275	206	C_2-Phenanthrene/C_2-Anthracene	11
2294	226	C_3-Dibenzothiophene	23

continued...

Table 6.1.1. Concluded.

Scan	M.W.	Compound	ppb
2325	226	Benzo(ghi)flouranthene	21
2340	226	C_2-Dibenzothiophene	18
2358	226	C_3-Dibenzothiophene	13
2364	226	C_3-Dibenzothiophene	16
2386	226	C_3-Dibenzothiophene	16
2436	220	C_3-Phenanthrene/C_3-Anthracene	12
2519	220	C_3-Phenanthrene/C_3-Anthracene	17
2616	234	C_4-Phenanthrene/C_4-Anthracene	5
2653	234	C_4-Phenanthrene/C_4-Anthracene	17
2702	234	Benzonaphthothiophene	13
2735	234	C_4-Phenanthrene/C_4-Anthracene	6
2805	228	Chrysene + Triphenylene	10

Table 6.1.2. SHOP treater water extractable aromatics, 1983 May.

Scan	M.W.	Compound	ppb
498	154	1,1'-Biphenyl	37
509	162	C_2-Benzo(b)thiophene	20
531	156	C_2-Naphthalene	242
532	162	C_2-Benzo(b)thiophene	13
551	156	C_2-Naphthalene	304
556	156	C_2-Naphthalene	177
563	162	C_2-Benzo(b)thiophene	15
578	156	C_2-Naphthalene	125
583	156	C_2-Naphthalene	69
600	156	C_2-Naphthalene	90
660	168	C_1-Biphenyl	11
673	170	C_3-Naphthalene	92
674	176	C_3-Benzo(b)thiophene	37
682	170	C_3-Naphthalene	28
689	168	Dibenzofuran	45
698	176	C_3-Benzo(b)thiophene	80
700	170	C_3-Naphthalene	37
706	170	C_3-Naphthalene	106
713	170	C_3-Naphthalene	160
724	176	C_3-Benzo(b)thiophene	55
737	170	C_3-Naphthalene	140
741	170	C_3-Naphthalene	95
763	170	C_3-Naphthalene	106
766	170	C_3-Naphthalene	81
788	170	C_3-Naphthalene	27
790	166	Fluorene	48
797	176	C_3-Benzo(b)thiophene	10
799	170	C_3-Naphthalene	72
818	184	C_4-Naphthalene	41
819	168	C_1-Biphenyl	20
820	190	C_4-Benzo(b)thiophene	43
835	190	C_4-Benzo(b)thiophene	18
846	184	C_4-Naphthalene	38
851	182	C_1-Dibenzofuran	27
854	184	C_4-Naphthalane	28
861	184	C_4-Naphthalene	26
864	190	C_4-Benzo(b)thiophene	16
865	182	C_2-Biphenyl	50
865	184	C_4-Naphthalene	25
870	182	C_1-Dibenzofuran	18
879	190	C_4-Benzo(b)thiophene	9
897	184	C_4-Naphthalene	40
919	190	C_4-Benzo(b)thiophene	10
929	184	C_4-Naphthalene	57
940	204	C_5-Benzo(b)thiophene	8
946	190	C_4-Benzo(b)thiophene	12
951	204	C_5-Benzo(b)thiophene	5
954	184	C_4-Naphthalene	46
959	204	C_5-Benzo(b)thiophene	12
961	184	C_4-Naphthalene	24

continued...

Table 6.1.2. Continued.

Scan	M.W.	Compound	ppb
966	180	C_1-Fluorene	15
967	204	C_5-Benzo(b)thiophene	7
970	180	1-Methylfluorene	13
979	180	2-Methylfluorene	52
989	196	C_3-Biphenyl	19
993	204	C_5-Benzo(b)thiophene	10
996	180	C_1-Fluorene	13
1000	184	C_4-Naphthalene	18
1022	182	C_2-Biphenyl	14
1026	184	C_4-Naphthalene	27
1035	196	C_3-Biphenyl	21
1049	184	Dibenzothiophene	129
1090	178	Phenanthrene	168
1126	194	C_2-Fluorene	7
1150	194	C_2-Fluorene	17
1158	194	C_2-Fluorene	21
1162	194	C_2-Fluorene	12
1170	194	C_2-Fluorene	25
1191	194	C_2-Fluorene	12
1203	198	C_1-Dibenzothiophene	226
1212	210	C_4-Biphenyl	13
1220	210	C_4-Biphenyl	12
1225	196	C_3-Biphenyl	16
1235	198	C_1-Dibenzothiophene	158
1267	192	C_1-Phenanthrene	60
1269	198	C_1-Dibenzothiophene	154
1275	192	C_1-Phenanthrene/C_1-Anthracene	70
1303	192	C_1-Phenanthrene/C_1-Anthracene	116
1307	210	C_4-Biphenyl	11
1308	208	C_3-Fluorene	9
1310	192	1-Methylphenanthrene	75
1325	208	C_3-Fluorene	4
1328	208	C_3-Fluorene	7
1337	208	C_3-Fluorene	12
1345	208	C_3-Fluorene	10
1345	212	C_2-Dibenzothiophene	28
1356	212	C_2-Dibenzothiophene	74
1362	208	C_3-Fluorene	3
1364	208	C_3-Fluorene	4
1375	208	C_3-Fluorene	10
1378	212	C_2-Dibenzothiophene	54
1388	212	C_2-Dibenzothiophene	135
1395	212	C_2-Dibenzothiophene	14
1402	208	C_3-Fluorene	6
1417	212	C_2-Dibenzothiophene	51
1422	208	C_3-Fluorene	8
1423	212	C_2-Dibenzothiophene	99
1432	206	C_2-Phenanthrene/C_2-Anthracene	25
1444	212	C_2-Dibenzothiophene	49
1447	206	C_2-Phenanthrene/C_2-Anthracene	25
1450	212	C_2-Dibenzothiophene	22
1472	206	C_2-Phenanthrene/C_2-Anthracene	98

continued...

Table 6.1.2. Concluded.

Scan	M.W.	Compound	ppb
1481	206	C_2-Phenanthrene/C_2-Anthracene	46
1490	206	C_2-Phenanthrene/C_2-Anthracene	35
1490	226	C_3-Dibenzothiophene	26
1506	206	C_3-Phenanthrene/C_2-Anthracene	26
1524	226	C_3-Dibenzothiophene	51
1557	226	C_3-Dibenzothiophene	48
1570	226	C_3-Dibenzothiophene	37
1575	202	Pyrene	11
1589	226	C_3-Dibenzothiophene	23
1594	226	C_3-Dibenzothiophene	36
1603	220	C_3-Phenanthrene/C_3-Anthracene	11
1612	240	C_4-Dibenzothiophene	5
1617	226	C_3-Dibenzothiophene	31
1631	220	C_3-Phenanthrene/C_3-Anthracene	17
1631	240	C_4-Dibenzothiophene	10
1643	220	C_3-Phenanthrene/C_3-Anthracene	34
1643	226	C_3-Dibenzothiophene	10
1652	240	C_4-Dibenzothiophene	6
1654	226	C_3-Dibenzothiophene	9
1659	220	C_3-Phenanthrene/C_3-Anthracene	7
1666	220	C_3-Phenanthrene/C_3-Anthracene	18
1684	240	C_4-Dibenzothiophene	12
1694	240	C_4-Dibenzothiophene	5
1709	240	C_4-Dibenzothiophene	4
1716	216	Benzo(a)fluorene	2
1749	220	C_3-Phenanthrene/C_3-Anthracene	22
1776	216	C_1-Pyrene	4
1845	234	C_4-Phenanthrene/C_4-Anthracene	4
1932	234	C_4-Phenanthrene/C_4-Anthracene	12
2032	228	Chrysene/Triphenylene	10
2178	242	C_1-Chrysene/C_1-Triphenylene	6

Table 6.1.3. SHOP treater water extractable aromatics, 1984 February.

Scan	M.W.	Compound	ppb
505	156	C_2-Naphthalene	170
509	156	C_2-Naphthalene	110
530	156	C_2-Naphthalene	72
535	156	C_2-Naphthalene	43
551	156	C_2-Naphthalene	51
622	170	C_3-Naphthalene	86
629	170	C_3-Naphthalene	21
637	168	C_1-Biphenyl	21
644	176	C_3-Benzo(b)thiophene	83
647	170	C_3-Naphthalene	41
653	170	C_3-Naphthalene	110
659	170	C_3-Naphthalene	150
671	176	C_3-Benzo(b)thiophene	50
683	170	C_3-Naphthalene	210
710	170	C_3-Naphthalene	160
733	166	Fluorene	27
733	190	C_4-Benzo(b)thiophene	14
742	170	C_3-Naphthalene	64
762	184	C_4-Naphthalene	49
764	190	C_4-Benzo(b)thiophene	65
770	170	C_3-Naphthalene	18
772	184	C_4-Naphthalene	18
778	190	C_4-Benzo(b)thiophene	25
779	184	C_4-Naphthalene	14
789	184	C_4-Naphthalene	51
794	182	C_2-Biphenyl	25
797	184	C_4-Naphthalene	31
804	184	C_4-Naphthalene	31
806	190	C_4-Benzo(b)thiophene	21
808	184	C_4-Naphthalene	31
813	182	C_2-Biphenyl	12
827	184	C_4-Naphthalene	32
831	190	C_4-Benzo(b)thiophene	9.3
839	184	C_4-Naphthalene	53
846	184	C_4-Naphthalene	8.4
871	184	C_4-Naphthalene	54
881	204	C_5-Benzo(b)thiophene	22
895	184	C_4-Naphthalene	55
901	204	C_5-Benzo(b)thiophene	24
902	184	C_4-Naphthalene	28
907	180	C_1-Fluorene	18
919	180	C_1-Fluorene	33
929	196	C_3-Biphenyl	23
933	204	C_5-Benzo(b)thiophene	16
962	182	C_2-Biphenyl	11
966	196	C_3-Biphenyl	11
971	218	C_6-Benzo(b)thiophene	10

continued...

Table 6.1.3. Continued.

Scan	M.W.	Compound	ppb
974	196	C_3-Biphenyl	25
987	184	Dibenzothiophene	84
987	196	C_3-Biphenyl	16
996	196	C_3-Biphenyl	13
1004	218	C_6-Benzo(b)thiophene	12
1009	196	C_3-Biphenyl	24
1009	218	C_6-Benzo(b)thiophene	5.9
1023	218	C_6-Benzo(b)thiophene	7.4
1027	178	Phenanthrene	120
1028	218	C_6-Benzo(b)thiophene	9.6
1068	218	C_6-Benzo(b)thiophene	13
1087	194	C_2-Fluorene	12
1095	194	C_2-Fluorene	20
1100	194	C_2-Fluorene	4.1
1107	194	C_2-Fluorene	18
1127	194	C_2-Fluorene	6.8
1139	198	C_1-Dibenzothiophene	230
1148	210	C_4-Biphenyl	20
1161	196	C_3-Biphenyl	20
1171	196	C_3-Biphenyl	8.4
1171	198	C_1-Dibenzothiophene	160
1184	196	C_3-Biphenyl	13
1189	210	C_4-Biphenyl	8.4
1195	198	C_1-Dibenzothiophene	2.2
1203	192	C_1-Phenanthrene	44
1204	198	C_1-Dibenzothiophene	180
1211	192	C_1-Phenanthrene	56
1238	192	C_1-Phenanthrene	96
1242	210	C_4-Biphenyl	15
1243	208	C_3-Fluorene	3.2
1246	192	C_1-Phenanthrene	61
1274	208	C_3-Fluorene	3.2
1280	208	C_3-Fluorene	6.2
1280	212	C_2-Dibenzothiophene	29
1290	212	C_2-Dibenzothiophene	87
1300	208	C_3-Fluorene	2.1
1302	212	C_2-Dibenzothiophene	5.0
1311	208	C_3-Fluorene	6.2
1313	212	C_3-Fluorene	60
1323	212	C_2-Dibenzothiophene	200
1323	208	C_3-Fluorene	0.74
1327	208	C_3-Fluorene	1.3
1337	208	C_3-Fluorene	3.1
1346	212	C_2-Dibenzothiophene	9.6
1347	210	C_4-Biphenyl	10
1356	212	C_2-Dibenzothiophene	210

continued...

Table 6.1.3. Continued.

Scan	M.W.	Compound	ppb
1357	208	C_3-Fluorene	3.4
1367	206	C_2-Phenanthrene	17
1371	206	C_2-Phenanthrene	1.9
1379	212	C_2-Dibenzothiophene	63
1382	206	C_2-Phenanthrene	5.5
1384	212	C_2-Dibenzothiophene	26
1388	206	C_2-Phenanthrene	3.0
1407	206	C_2-Phenanthrene	100
1417	206	C_2-Phenanthrene	46
1424	226	C_3-Dibenzothiophene	42
1425	206	C_2-Phenanthrene	34
1434	206	C_2-Phenanthrene	2.5
1440	206	C_2-Phenanthrene	9.0
1459	226	C_3-Dibenzothiophene	88
1481	206	C_2-Phenanthrene	3.3
1491	226	C_3-Dibenzothiophene	81
1504	226	C_3-Dibenzothiophene	75
1516	226	C_3-Dibenzothiophene	2.7
1523	226	C_3-Dibenzothiophene	37
1528	226	C_3-Dibenzothiophene	85
1537	220	C_3-Phenanthrene	4.4
1541	220	C_3-Phenanthrene	3.2
1551	226	C_3-Dibenzothiophene	60
1565	220	C_3-Phenanthrene	36
1568	240	C_4-Dibenzothiophene	23
1576	226	C_3-Dibenzothiophene	16
1577	220	C_3-Phenanthrene	58
1581	240	C_4-Dibenzothiophene	14
1586	240	C_4-Dibenzothiophene	14
1587	226	C_3-Dibenzothiophene	9.7
1593	220	C_3-Phenanthrene	7.1
1600	220	C_3-Phenanthrene	29
1602	226	C_3-Dibenzothiophene	3.0
1617	240	C_4-Dibenzothiophene	22
1621	240	C_4-Dibenzothiophene	21
1638	220	C_3-Phenanthrene	4.9
1648	240	C_4-Dibenzothiophene	2.9
1648	216	C_1-Pyrene	5.2
1680	240	C_4-Dibenzothiophene	2.9
1681	220	C_3-Phenanthrene	26
1690	254	C_5-Dibenzothiophene	11
1706	216	Benzo(a)fluorene	4.9
1707	254	C_5-Dibenzothiophene	21
1717	240	C_4-Dibenzothiophene	3.3
1722	240	C_4-Dibenzothiophene	3.7
1739	240	C_4-Dibenzothiophene	6.6
1740	234	C_4-Phenanthrene	3.2
1744	234	C_4-Phenanthrene	1.9

continued...

Table 6.1.3. Concluded.

Scan	M.W.	Compound	ppb
1778	234	C_4-Phenanthrene	9.2
1778	254	C_5-Dibenzothiophene	8.1
1805	230	C_2-Pyrene/C_1-Benzofluorene	1.1
1810	230	C_2-Pyrene/C_1-Benzfluorene	2.7
1812	234	C_4-Phenanthrene	3.2
1815	230	C_2-Pyrene/C_1-Benzfluorene	4.5
1835	230	C_2-Pyrene/C_1-Benzfluorene	4.4
1842	230	C_2-Pyrene/C_1-Benzfluorene	3.2
1860	234	C_4-Phenanthrene	23
1893	234	C_4-Phenanthrene	11
1894	230	C_2-Pyrene/C_1-Benzfluorene	5.2
1960	228	Chrysene/Triphenylene	35
1983	244	C_3-Pyrene/C_2-Benzfluorene	7.4
1994	248	C_5-Phenanthrene	28
2003	244	C_3-Pyrene/C_2-Benzfluorene	37
2022	248	C_5-Phenanthrene	45
2037	248	C_5-Phenanthrene	11
2041	244	C_3-Pyrene/C_2-Benzfluorene	8.9
2046	248	C_5-Phenanthrene	10
2058	248	C_5-Phenanthrene	69
2078	244	C_3-Pyrene/C_2-Benzfluorene	6.7
2085	248	C_5-Phenanthrene	21
2108	242	C_1-Chrysene/C_1-Triphenylene	21
2121	242	C_1-Chrysene/C_1-Triphenylene	6.5
2143	262	C_6-Phenanthrene/C_6-Anthracene	15
2151	262	C_6-Phenanthrene/C_6-Anthracene	8.1
2158	262	C_6-Phenanthrene/C_6-Anthracene	7.7
2173	262	C_6-Phenanthrene/C_6-Anthracene	21
2182	262	C_6-Phenanthrene/C_6-Anthracene	34
2187	262	C_6-Phenanthrene/C_6-Anthracene	23
2196	262	C_6-Phenanthrene/C_6-Anthracene	18
2202	262	C_6-Phenanthrene/C_6-Anthracene	8.1
2211	262	C_6-Phenanthrene/C_6-Anthracene	54
2222	262	C_6-Phenanthrene/C_6-Anthracene	3.9
2233	262	C_6-Phenanthrene/C_6-Anthracene	19
2250	256	C_2-Chrysene/C_2-Triphenylene	7.2
2274	256	C_2-Chrysene/C_2-Triphenylene	6.1
2313	276	C_7-Phenanthrene/C_7-Anthracene	29
2317	276	C_7-Phenanthrene/C_7-Anthracene	20
2326	276	C_7-Phenanthrene/C_7-Anthracene	9.0
2340	276	C_7-Phenanthrene/C_7-Anthracene	95
2354	276	C_7-Phenanthrene/C_7-Anthracene	27
2354	256	C_2-Chrysene/C_2-Triphenylene	9.8
2364	276	C_7-Phenanthrene/C_7-Anthracene	15
2386	276	C_7-Phenanthrene/C_7-Anthracene	31

Table 6.1.4. SHOP treater water acidic components, 1983 January.

Scan	M.W.	Compound	ppb
356	136	C_3-Phenol	0.26
369	136	C_3-Phenol	0.56
391	136	C_3-Phenol	0.43
405	136	C_3-Phenol	1.4
431	150	C_4-Phenol	7.7
460	150	C_4-Phenol	0.72
461	136	C_3-Phenol	1.8
500	150	C_4-Phenol	0.51
506	150	C_2-Benzoic acid	0.66
524	150	C_4-Phenol	0.67
559	150	C_4-Phenol	0.35
576	150	C_2-Benzoic acid	1.9
598	150	C_4-Phenol	0.61
618	150	C_2-Benzoic acid	2.8
682	164	C_3-Benzoic acid	3.5
721	164	C_3-Benzoic acid	2.9
739	150	C_4-Phenol	0.66
743	150	C_2-Benzoic acid	0.63
770	164	C_3-Benzoic acid	7.5
913	192	C_5-Benzoic acid	5.0
940	192	C_7-Phenol, or C_5-Benzoic acid	8.2
979	192	C_7-Phenol, or C_5-Benzoic acid	3.0
1045	192	C_7-Phenol	5.4
1051	206	C_8-Phenol, or C_6-Benzoic acid	4.9
1096	206	C_8-Phenol, or C_6-Benzoic acid	5.4
1116	206	C_8-Phenol, or C_6-Benzoic acid	3.2
1137	206	C_8-Phenol, or C_6-Benzoic acid	2.2
1173	220	C_9-Phenol, or C_7-Benzoic acid	3.3
1288	220	C_7-Benzoic acid	4.0
1289	234	C_{10}-Phenol, or C_8-Benzoic acid	2.8
1299	220	C_9-Phenol, or C_7-Benzoic acid	6.2
1311	204	C_9-Benzene	7.0
1329	234	C_8-Benzoic acid	0.76
1336	220	C_9-Phenol, or C_7-Benzoic acid	3.3
1433	234	C_{10}-Phenol, or C_8-Benzoic acid	1.9
1483	234	C_{10}-Phenol, or C_8-Benzoic acid	12
1809	228	C_3-Dihydroxybiphenyl	3.9

Table 6.1.5. SHOP treater water acidic components, 1984 February.

Scan	M.W.	Compound	ppb
328	136	C_3-Phenol	0.66
342	136	C_1-Benzoic acid	1.3
358	150	C_4-Phenol	2.0
365	150	C_4-Phenol	0.84
370	136	C_1-Benzoic acid	68
372	150	C_4-Phenol	2.6
392	150	C_4-Phenol	2.3
423	150	C_2-Benzoic acid	1.2
454	164	C_5-Phenol	2.1
462	150	C_2-Benzoic acid	22
468	150	C_2-Benzoic acid	6.6
484	150	C_2-Benzoic acid	36
554	150	C_2-Benzoic acid	19
589	164	C_5-Phenol	5.4
637	164	C_3-Benzoic acid	2.0
641	182	C_4-Dihyroxyphenol	3.7
649	164	C_5-Phenol	1.5
700	178	C_6-Phenol	5.0
718	196	C_1-Fluorenol	0.43
926	172	Naphthalene carboxylic acid	5.9
956	172	Naphthalene carboxylic acid	1.2
963	192	C_5-Benzoic acid	1.3
1066	186	C_1-Naphthalene carboxylic acid	3.9
1076	186	C_1-Naphthalene carboxylic acid	0.39
1085	186	C_1-Naphthalene carboxylic acid	1.0
1104	186	C_1-Naphthalene carboxylic acid	0.78
1118	186	C_1-Naphthalene carboxylic acid	2.0
1140	186	C_1-Naphthalene carboxylic acid	0.58
1145	158	C_1-Naphthalenol	0.96
1239	200	C_2-Naphthalene carboxylic acid	0.66
1253	200	C_2-Naphthalene carboxylic acid	0.59
1265	200	C_2-Naphthalene carboxylic acid	0.48
1273	200	C_2-Naphthalene carboxylic acid	0.36
1294	200	C_2-Naphthalene carboxylic acid	0.66
1372	214	C_3-Naphthalene carboxylic acid	0.37

Table 6.1.6. SHOP treater water nitrogen components, 1984 February.

Scan	M.W.	Compound	ppb
288	136	C_4-Pyrazine	0.10
309	150	C_3-Diaminobenzene or C_5-Pyrazine	0.15
315	136	C_4-Pyrazine	0.35
335	150	C_3-Diaminobenzene or C_5-Pyrazine	0.23
359	135	C_4-Pyridine	0.10
395	164	C_4-Diaminobenzene or C_6-Pyrazine	0.10
425	136	C_2-Diaminobenzene or C_4-Pyrazine	0.10
463	164	C_4-Diaminobenzene or C_6-Pyrazine	0.10
694	177	C_6-Aniline or C_7-Pyridine	0.17
709	185	C_4-Quinoline	0.10
723	185	C_4-Quinoline	0.12
784	199	C_5-Quinoline	0.10
824	199	C_5-Quinoline	0.21
840	199	C_5-Quinoline	0.11
861	199	C_5-Quinoline	0.10
878	199	C_5-Quinoline	0.11
908	199	C_5-Quinoline	0.10
934	199	C_5-Quinoline	0.10
959	199	C_5-Quinoline	0.10
964	199	C_5-Quinoline	0.10
976	213	C_6-Quinoline	0.22
979	213	C_5-Naphthylamine	0.10
987	213	C_6-Quinoline	0.10
1014	213	C_6-Quinoline	0.10
1023	213	C_6-Quinoline	0.10
1050	213	C_6-Quinoline	0.30
1055	213	C_5-Naphthylamine	0.58
1072	213	C_6-Quinoline	0.10
1084	213	C_6-Quinoline	0.10
1093	213	C_6-Quinoline	0.21
1125	227	C_7-Quinoline	0.26
1157	227	C_7-Quinoline	0.10
1337	207	C_1-Aminophenanthrene/ C_1-Aminoanthracene	0.32
1350	207	C_2-Benzoquinoline	0.12
1495	221	C_3-Benzoquinoline	0.13
1509	221	C_3-Benzoquinoline	0.10
1521	221	C_3-Benzoquinoline	0.13
1544	221	C_3-Benzoquinoline	0.10
1615	221	C_3-Benzoquinoline	0.10

APPENDIX 6.2

Volatile constituents of Gregoire Lake-produced waters.

Table 6.2.1. GP20 volatiles, 1981 January (21 ppm).

Scan	M.W.	Compound	ppm^a
239			0.560
248			0.081
281			0.097
315	88	2-methyl-2-butanol	0.032
338	78	benzene	0.234
350			0.032
362	98	1,3-dimethyl cyclopentane	0.023
371	98	1,2-dimethyl cyclopentane	0.087
386			0.068
427	98	methyl cyclohexane	0.206
451	98	ethyl cyclopentane	0.036
463	112	1,2,4-trimethyl cyclopentane	0.052
481	112	1,2,3-trimethyl cyclopentane	0.067
520	112	1,1,2-trimethyl cyclopentane	0.019
536	92	methyl benzene	0.849
554	112	1,2-dimethyl cyclohexane	0.076
590	112	1,1-dimethyl cyclohexane	0.018
600	112	1-ethyl-3-methyl cyclopentane	0.014
613	112	1-ethyl-2-methyl cyclopentane	0.059
634	112	1,4-dimethyl cyclohexane	0.101
659	114	octane	0.250
675	112	dimethyl cyclohexane	0.047
699	126	(2-methylpropyl)cyclopentane	0.011
739	116	5-methyl-1-hexanol	0.009
801			0.033
807	112	dimethyl cyclohexane	0.028
818	128	2,6-dimethyl heptane	0.177
825	112	ethyl cyclohexane	0.323
835	126	1,1,3-trimethyl cyclohexane	0.605
851	126	1-ethyl-1-methyl: cyclohexane	0.173
882	126	1,3,5-trimethyl cyclohexane	0.283
907	128	2,3-dimethyl heptane	0.128
924	106	ethyl benzene	0.111
939	128	2,4-dimethyl heptane	0.134
957	106	1,3-dimethyl benzene	1.391
966	128	3-methyl octane	0.448
989	126	1,1,3-trimethyl cyclohexane	0.101
1015			0.590
1038	106	1,4-dimethyl benzene	0.870
1071	128	nonane	1.484
1085			0.172
1094	126	1-ethyl-4-methyl cyclohexane	0.030
1125	124	1-methyl-octohydro pentalene	0.585
1152	120	(1-methylethyl)benzene	0.136
1166	126	propyl cyclohexane	0.453
1186	142	3-methyl nonane	0.613
1211	142	3-ethyl-2-methyl heptane	0.691
1224	124	cyclopropyl cyclohexane	0.107
1240	140	diethyl cyclohexane	0.036
1258	140	3,7-dimethyl-1-octene	0.470
1288	120	1-ethyl-3-methyl benzene	0.391
1296			0.123
1313	120	1,2,3-trimethyl benzene	0.124
1323			0.276
1333			0.044
1353	120	1-ethyl-4-methyl benzene	0.064
1361			0.097
1369	140	(2-methylpropyl)cyclohexane	0.222
1389	140	4-ethyl-3-octene	0.014
1405	120	1,3,5-trimethyl benzene	0.396
1427	120	decane	0.577
1456			0.012
1476			0.015
1481			0.010
1511	156	4-methyl decane	0.255
1526			0.012
1543	140	butyl cyclohexane	0.057
1552			0.005
1570			0.038
1587	154	5-methyl-1-decene	0.019
1632	138	decahydro naphthalene	0.010
1641			0.019
1669			0.042
1692			0.013
1713			0.051

continued...

Table 6.2.1. Concluded.

Scan	M.W.	Compound	ppm[a]
1750			0.009
1768			0.012
1811	156	undecane	0.111
1854			0.010
1878			0.013
1918			0.041
2124			0.004
2137	166	2,6-dimethyl-decahydro naphthalene	0.010
2172	128	naphthalene	0.081
2210			0.005
2222			0.017
2249			0.004
2277			0.031
2315			0.027
2365			0.004
2379			0.003
2423			0.010
2436			0.006
2440			0.005
2444			0.007
2470			0.016
2508	146	6-methyl-1,2,3,4-tetrahydro naphthalene	0.026
2523			0.029
2549			0.022
2574			0.008
2593			0.007
2633	142	1-methyl naphthalene	0.407
2700	142	2-methyl naphthalene	0.209
2726			0.002
2731			0.003
2804			0.003
2821			0.019
2900			0.007
2924			0.008
2949			0.010
2989			0.003
3034			0.152
3044	198	tetradecane	0.067
3089	156	1,2-dimethyl naphthalene	0.004
3093	156	1,7-dimethylnaphthalene	0.003
3154			0.010
3158			0.007
3168			0.006
3224			0.005
3330			0.003
3234			0.005
3280			0.002
3290			0.008

[a] Approximate concentration based on a total volatile carbon content of 21 ppm.

Table 6.2.2. GP 20 volatiles, 1981 March (10 ppm).

Scan	M.W.	Compound	ppm[a]
240	56	2-butene	0.009
253			0.025
270			0.016
283	86	3-methyl pentane	0.016
301			0.015
328	78	benzene	0.658
346			0.014
352	98	1,3-dimethyl cyclopentane	0.037
362			0.046
387			0.014
395	98	methyl cyclohexane	0.018
412	98	ethyl cyclopentane	0.007
421	112	1,2,4-trimethylcylopentane	0.024
434	112	1,2,3-trimethyl cyclopentane	0.035
468	128	4-ethyl-2-methyl hexane	0.042
477	92	methyl benzene	0.204
486	128	3-ethyl-2-methyl hexane	0.048
498	112	1,3-dimethyl cyclohexane	0.095
517	112	1,1-dimethyl cyclohexane	0.007
522	112	1-ethyl-3-methyl cyclopentane	0.009
532	112	1-ethyl-2-methyl cyclopentane	0.027
548	112	1,4-dimethyl cyclohexane	0.037
556	114	octane	0.106
570	112	dimethyl cyclohexane	0.018
602			0.010
653	128	2,6-dimethyl heptane	0.045
668	112	ethyl cyclohexane	0.034
681	126	1,1,3-trimethyl cyclohexane	0.279
705			0.025
733			0.065
745	126	1,3,5-trimethyl cyclohexane	0.105
775	128	2,3-dimethyl heptane	0.053
800	106	ethyl benzene	0.083
821			0.045
845	106	1,3-dimethyl benzene	0.516
855	126	2-ethyl-1,1-dimethyl cyclopentane	0.183
872	126	1,1,2-trimethyl cyclohexane	0.073
889	126	1-ethyl-2-methyl cyclohexane	0.148
904	106	1,4-dimethyl benzene	0.930
923			0.076
929	128	nonane	0.106
937			0.031
946			0.066
1000	124	1-methyl octahydro pentalene	0.162
1048			0.175
1082	142	3-methyl nonane	0.124
1114			0.354
1146			0.013
1168	140	2,2,5,5-tetramethyl-3-hexane	0.408
1213	120	1-ethyl-3-methyl benzene	0.520
1240	120	1,2,3-trimethyl benzene	0.336
1292	120	1-ethyl-4-methyl benzene	0.153
1313			0.033
1356	120	1,3,5-trimethyl benzene	0.830
1386	142	decane	0.133
1480	120	1,2,4-trimethyl benzene	0.201
1516			0.011
1563			0.020
1611	138	decahydro naphthalene	0.013
1657			0.015
1704			0.019
1817	156	5-methyl decane	0.021
1926	152	2-methyl decahydro naphthalene	0.010
2043	134	1,2,3,5-tetramethyl benzene	0.027
2119			0.002
2144			0.001
2151			0.002
2157			0.002
2189	128	naphthalene	0.012
2198			0.015
2223			0.003
2228			0.001
2244			0.014
2298			0.009
2337			0.006
2492			0.002

Table 6.2.3. GP21 volatiles, 1981 February (11 ppm).

Scan	M.W.	Compound	ppm[a]
241			0.111
245			0.248
285	88	2-methyl-2-butanol	0.069
299	78	benzene	1.103
317	98	1,2-dimethyl cyclopentane	0.126
324	100	heptane	0.083
349	98	methyl cyclohexane	0.336
361	98	ethyl cyclopentane	0.043
367	112	1,2,4-trimethyl cyclopentane	0.083
377	112	1,2,3-trimethyl cyclopentane	0.079
400	128	4-ethyl-2-methyl hexane	0.113
408	92	methyl benzene	0.533
424	112	1,2-dimethyl cyclohexane	0.288
440			0.032
447	112	1-ethyl-2-methyl cyclopentane	0.057
462			0.397
475	112	1,3-dimethyl cyclohexane	0.043
497			0.015
513			0.010
530	128	2,4-dimethyl heptane	0.076
545	112	ethyl cyclohexane	0.178
554	126	1,1,3-trimethyl cyclohexane	0.680
569			0.088
588			0.114
598	126	1,3,5-trimethyl cyclohexane	0.200
614	128	2,3-dimethyl heptane	0.086
644	128	2,6-dimethyl heptane	0.069
654	110	octahydro pentalene	0.006
668	106	ethyl benzene	0.348
678	126	butyl cyclopentane	0.115
708	126	1,1,2-trimethyl cyclohexane	0.083
725			0.031
734	126	1-ethyl-1-methyl cyclohexane	0.084
753	124	bicycle-3-3-2-nonane	0.045
764	106	1,3-dimethyl benzene	0.054
802			0.148
825	126	1-ethyl-2-methyl cyclohexane	0.056
841	126	1-ethyl-4-methyl cyclohexane	0.006
853			0.033
871	124	1-methyl-octahydro pentalene	0.339
894			0.140
926	142	3-methyl nonane	0.134
960			0.511
1000	140	diethyl cyclohexane	0.019
1024	140	2,2,5,5-tetramethyl-3-hexane	0.371
1084			0.030
1105	140	5-methyl nonene	0.054
1121			0.063
1135	140	4-decene	0.043
1161			0.034
1197			0.022
1210			0.006
1238	120	1,2,4-trimethyl benzene	0.238
1276			0.055
1386			0.140
1424			0.012
1475	154	2-propyl octene	0.034
1537	134	1-phenyl-1-propanone	0.014
1541			0.011
1583			0.022
1635			0.040
1764	156	2,5-dimethyl nonane	0.057
2122			0.003
2151			0.002
2155			0.001
2222			0.004
2229			0.003
2236			0.001
2283			0.005
2311			0.003
2537			0.002
2672			0.009
2687			0.006
2985			0.002
2992			0.001
3089			0.010

[a] Approximate concentration based on a total volatile carbon content of 11 ppm.

Table 6.2.4. GP21 volatiles, 1981 March (21 ppm).

Scan	M.W.	Compound	ppm[a]
235			0.381
248	74	2-methyl-2-propanol	3.806
311			0.182
316	70	2-methyl-2-butene	0.284
327	78	benzene	1.284
338	98	1,1-dimethyl cyclopentane	0.144
350			0.027
357	98	1,2-dimethyl cyclopentane	0.107
371	100	heptane	0.049
381			0.031
396			0.072
411	112	1-ethyl-1-methyl cyclopentane	0.299
445	112	1,2,3-trimethyl(, ,)cyclopentane	0.055
462	112	1,2,3-trimethyl(, ,)cyclopentane	0.093
500	112	1,1,2-trimethyl cyclopentane	0.061
516	92	methyl benzene	0.298
529	126	1,1,3,4-tetramethyl cyclopentane	0.086
542	112	1,2-dimethyl cyclohexane	0.142
566	112	1,1-dimethyl cyclohexane	0.055
586			0.066
605	112	1,4-dimethyl cyclohexane	0.080
618			0.092
633			0.049
650			0.050
675	116	4-methyl-1-hexanol	0.047
734			0.026
750	126	1,1,3,3-tetramethyl cyclopentane	0.043
766			0.032
787	126	1,1,3-trimethyl cyclohexane	0.884
828			0.113
855			0.158
861	126	1,3,5-trimethyl cyclohexane	0.138
884	128	2,3-dimethyl heptane	0.108
897			0.029
913			0.049
939	126	1,2,3-trimethyl cyclohexane	0.231
965	126	1,1,2-trimethyl cyclohexane	0.295
979			0.110
1004	124	bicyclo-3-3-1-nonane	0.109
1014			0.072
1042			0.057
1046			0.058
1056			0.105
1074			0.179
1113			0.064
1123			0.035
1150	140	2,2,5,5-tetramethyl-3-hexene	0.092
1163			0.091
1178			0.066
1202	142	3-ethyl-2-methyl heptane	0.358
1251			0.825
1269			0.105
1312			0.119
1323			0.009
1331			0.054
1352			0.087
1388			0.028
1598			0.069
1726			0.023
1732			0.016
2055	134	1-methyl-2-(1-methylethyl)benzene	0.137
2218			0.012
2229			0.029
2259			0.005
2271			0.028
2305			0.010
2555			0.020
2666			0.046
2679			0.010
2683			0.029
3448			0.011

[a] Approximate concentrations based on a volatile carbon content of 21 ppm

Table 6.2.5. GP21 volatiles, 1981 June (38 ppm).

Scan	M.W.	Compound	ppm[a]
244			0.486
269	58	oxetane	3.162
328			0.058
361	78	benzene	1.837
384	98	1,3-dimethyl-cis-cyclopentane	0.477
401	100	heptane	0.156
433	98	methyl cyclohexane	1.272
461	112	1,2,4-trimethyl cyclopentane	0.090
476	112	1,2,3-trimethyl cyclopentane	0.218
532	92	methyl benzene	3.540
542			1.612
597	128	2-methyl cyclohexanemethanol	0.039
608	70	ethenyl oxirane	0.373
616			0.333
703	128	2,2,5-trimethyl hexane	0.073
721	112	ethyl cyclohexane	0.370
733	126	1,1,3-trimethyl cyclohexane	1.578
787	126	1,1,3-trimethyl cyclohexane	1.236
800	128	2,3-dimethyl heptane	0.376
820	106	ethyl benzene	0.919
835	106	1,3-dimethyl benzene	5.882
859	126	1,2,4-trimethyl cyclohexane	0.254
878			0.153
889			0.098
904	106	1,4-dimethyl benzene	4.621
933			0.265
971	124	octahydro-cis-1H-indene	0.991
1002	126	1-ethyl-2-methyl cyclohexane	0.627
1022	142	2,2,5,5-tetramethyl hexane	0.373
1042	142	4-(1-methylethyl)heptane	1.105
1086	140	2,7-dimethyl-1-octene	0.970
1101			0.031
1125			0.163
1129			0.118
1140	120	2,4-dimethyl-2,3-heptadiene-5-yne	0.392
1144			0.482
1175			0.294
1231	120	(1-methylethyl)benzene	0.705
1237			0.476
1326	120	1,2,3-trimethyl benzene	0.095
1333			0.105
2505			0.045

[a] Approximate concentrations based on a volatile carbon content of 38 ppm.

Table 6.2.6. GP26 volatiles, 1981 February (21 ppm).

Scan	M.W.	Compound	ppm^{a}
245			0.594
272			0.161
286	84	2-methyl-1-pentene	0.003
307	78	benzene	0.200
325			0.039
333			0.041
359	98	methyl cyclohexane	0.022
379			0.010
411	128	4-ethyl-2-methyl hexane	0.020
419	92	methyl benzene	0.848
435	112	1,2-dimethyl cyclohexane	0.078
459	128	2,3,4-trimethyl hexane	0.016
541	128	2,4-dimethyl heptane	0.028
556	112	ethyl cyclohexane	0.109
564	126	1,1,3-trimethyl cyclohexane	0.038
582			0.008
600			0.017
610	126	1,3,5-trimethyl cyclohexane	0.056
626	128	2,3-dimethyl heptane	0.030
649	106	ethyl benzene	0.347
686	106	1,3-dimethyl benzene	1.159
782	126	3,4,4-trimethyl-2-hexene	0.199
828	106	1,4-dimethyl benzene	0.875
845	106	1,2-dimethyl benzene	0.069
864	128	nonane	0.865
879	126	1-ethyl-2-methyl cyclohexane	0.032
932	124	1-methyl-octahydro pentalene	0.221
963	120	(1-methylethyl)benzene	0.079
980	126	propyl cyclohexane	0.117
1008	142	3-methyl nonane	0.179
1037			0.234
1099	120	propyl benzene	0.334
1144	120	1-ethyl-3-methyl benzene	1.101
1174	120	1,2,3-trimethyl benzene	0.566
1222	120	1-ethyl-4-methyl benzene	0.336
1247			0.055
1293	120	1,3,5-trimethyl benzene	2.683
1317	142	decane	0.558
1348	134	(2-methylpropyl)benzene	0.018
1361	134	(1-methylpropyl)benzene	0.037
1379			0.021
1417	120	1,2,4-trimethyl benzene	1.260
1452	140	butyl cyclohexane	0.086
1473	118	1-ethenyl-2-methyl benzene	0.104
1488			0.054
1517			0.009
1554	138	decahydro naphthalene	0.110
1579	134	1-ethyl-3,5-dimethyl benzene	0.014
1601	156	isooctane	0.028
1615	134	1-methyl-4-propyl benzene	0.009
1631			0.023
1669	134	(1,1-dimethylethyl)benzene	0.025
1694			0.020
1705	132	2-butenyl benzene	0.052
1766	156	undecane	0.251
1787			0.010
1809	152	2-methyl-decahydro naphthalene	0.028
1841	134	1,2,3,5-tetramethyl benzene	0.032
1860	134	1,2,4,5-tetramethyl benzene	0.028
1885	170	4-methyl undecane	0.058
1918			0.013
1943	132	1-methyl-2-(2-propenyl)benzene	0.013
2005	134	2-ethyl-1,4-dimethyl benzene	0.178
2044	132	1,2,3,4,-tetrahydro naphthalene	0.052
2106	148	(1-1-dimethylpropyl)benzene	0.012
2118			0.014
2146	128	naphthalene	0.223
2172			0.007
2185	148	diethylmethyl benzene	0.004
2194			0.003
2215			0.053
2237			0.006
2261	148	2,4-dimethyl-1-(1-methylethyl)benzene	0.003
2273	184	2,6-dimethyl undecane	0.025
2297	148	(1,1-dimethyl ethyl)methyl benzene	0.005
2306			0.007

continued...

Table 6.2.6. Concluded.

Scan	M.W.	Compound	ppm[a]	Scan	M.W	Compound	ppm[a]
2310			0.006				
2329			0.004				
2372			0.008				
2380			0.011				
2403			0.003				
2422			0.003				
2439			0.010				
2453			0.001				
2471			0.006				
2498			0.004				
2505			0.003				
2531			0.014				
2552			0.009				
2604			0.002				
2627			0.001				
2653			0.064				
2666			0.012				
2673			0.032				
2725			0.006				
2742			0.001				
2972			0.007				
3077			0.007				

[a] Approximate concentration based on a total volatile carbon content of 21 ppm.

Table 6.2.7. GP26 volatiles, 1981 March (33 ppm).

Scan	M.W.	Compound	ppm[a]
254			4.046
288			0.852
299			0.181
303			0.272
321			0.028
332	78	benzene	1.028
340			0.230
357			0.317
369	86	3-pentanone	0.401
383			0.167
401	98	methyl cyclohexane	0.152
422			0.057
433	112	1,2,4-trimethyl cylopentane	0.027
441	100	4-methyl-2-pentanone	0.028
453	112	1,2,3-trimethyl cyclopentane	0.048
477	100	3-methyl-2-pentanone	0.073
520	92	methyl benzene	1.922
553	112	1,2-dimethyl cyclohexane	0.090
595			0.050
611	100	2-hexanone	0.141
631	112	1,3-dimethyl cyclohexane	0.095
644	114	octane	0.133
676			0.135
792	128	2,2,5-trimethyl hexane	0.036
813	112	ethyl cyclohexane	0.082
834	126	1,1,3-trimethyl cyclohexane	0.222
863			0.060
885	126	1,3,5-trimethyl cyclohexane	0.314
902	128	2,3-dimethyl heptane	0.073
919	106	ethyl benzene	0.606
935			0.013
954	106	1,3-dimethyl benzene	4.512
976	112	ethyl triophene	0.026
1010	126	1-ethyl-2-methyl cyclohexane	0.177
1035	106	1,4-dimethyl benzene	2.410
1063	128	nonane	0.812
1077			0.089
1122	124	1-methyl octahydro pentalene	0.418
1150	120	(1-methylethyl)benzene	0.122
1163	126	propyl cyclohexane	0.315
1183	142	3-methyl nonane	0.444
1209			0.635
1258			0.398
1288	120	1-ethyl-3-methyl benzene	0.286
1326			0.279
1363			0.113
1373	140	2-methyl-4-nonene	0.130
1411	120	1,3,5-trimethyl benzene	0.266
1433	142	decane	0.138
1462			0.013
1518	156	4-methyl decane	0.118
1555	140	butyl cylohexane	0.026
1562			0.006
1579			0.029
1598	154	5-methyl-1-decene	0.011
1645	138	decahydro naphthalene	0.015
1682			0.025
1727			0.057
1936			0.029
2141			0.006
2156			0.010
2178			0.015
2230			0.013
2241			0.002
2265			0.003
2269			0.002
2299			0.001
2306			0.002
2334			0.021
2390			0.004
2447			0.007
2458			0.006
2490			0.011
2508			0.003
2513			0.002
2568			0.013

continued...

Table 6.2.7. Concluded.

Scan	M.W.	Compound	ppm[a]	Scan	M.W	Compound	ppm[a]
2580			0.002				
2653			0.003				
2658			0.002				
2664			0.002				
2739			0.003				
2828			0.002				

[a] Approximate concentration based on a total volatile carbon content of 33 ppm.

Table 6.2.8. GP26 volatiles, 1981 (136 ppm).

Scan	M.W.	Compound	ppm[a]
228	46	oxybis methane	0.362
254	58	oxetane	26.289
300	72	3-methoxy-1-propene	5.096
365	78	benzene	12.765
407			1.479
424			3.968
518	100	2-hexanone	0.635
527			0.398
555	72	2-methyl butane	0.518
596	92	methyl benzene	25.213
642	98	3-methyl thiophene	1.670
693	100	4-methyl-2-pentanone	0.899
740			0.521
834			0.187
965	102	2-methyl-tetrahydro thiophene	0.910
983			0.099
988			0.306
1061	106	ethyl benzene	3.772
1123	106	1,3-dimethyl benzene	18.515
1172			0.321
1321	106	1,4-dimethyl benzene	9.999
1460			0.307
1465			0.076
1471	116	2,5-dimethyl-tetrahydro thiophene	0.157
1476			0.060
1492			0.172
1523	120	(1-methylethyl)benzene	0.824
1654	120	propyl benzene	0.529
1685	120	1-ethyl-3-methyl benzene	2.945
1711	120	1,2,3-trimethyl benzene	1.601
1756	120	1-ethyl-4-methyl benzene	1.521
1814	120	1,3,5-trimethyl benzene	7.657
1830	120	1,2,4-trimethyl benzene	0.596
1855			0.118
1930	120	1-ethyl-2,methyl benzene	1.587
1944			0.084
2169	134	diethyl benzene	0.027
2173	120	2-methyl benzaldehyde	0.026
2178			0.051
2184			0.121
2250			0.051
2265			0.028
2269			0.023
2278	146	2,2'-bi-1,3-dioxolane	0.056
3223			0.926
3336			0.104
3398			0.044
3412			0.052
3419			0.074
3455			0.092
3465			0.032
3474			0.092
3502			0.238
3784			0.152

[a] Approximate concentration based on a total volatile carbon content of 136 ppm.

Table 6.2.9. GP31 volatiles, 1981 February (242 ppm).

Scan	M.W.	Compound	ppm[a]
262			1.157
268			0.616
277			0.060
288	72	2-buten-1-ol	0.672
302			0.311
308	88	2-methyl-2-butanol	0.285
323	78	benzene	3.059
341	98	1,2-dimethyl cyclopentane	2.455
349	100	heptane	1.290
375	98	methylcyclohexane	4.808
387	98	ethyl cyclopentane	0.533
393	112	1,2,4-trimethyl cyclopentane	0.711
403	112	1,2,3-trimethyl cyclopentane	0.935
427	130	2-ethyl-4-methyl pentanol	0.604
435	92	methyl benzene	6.389
452	112	1,2-dimethyl cyclohexane	3.131
466	112	1,1-dimethyl cyclohexane	0.300
475	112	4-octene	0.557
489	112	1,4-dimethyl cyclohexane	2.977
503			1.331
558			0.184
573	112	ethyl cyclohexane	1.957
581	126	1,1,3-trimethyl cyclohexane	5.875
626	126	1,3,5-trimethyl cyclohexane	0.558
639			0.437
666			0.441
732			35.131
818			0.065
824			0.090
864	106	1,3-dimethyl benzene	19.973
883	128	nonane	4.221
900	126	1-ethyl-2-methyl cyclohexane	0.772
958	124	2-methyl-octahydro pentalene	4.671
989	120	(1-methylethyl)benzene	1.361
1003	126	propyl cyclohexane	0.881
1007	126	(1-methylethyl)cyclohexane	0.693
1028	142	2,6-dimethyl octane	0.937
1061	142	3-ethyl-2-methyl heptane	1.159
1072	124	1-methyl-octahydro pentalene	0.694
1117	120	propyl benzene	2.418
1156	120	1-ethyl-3-methyl benzene	6.983
1186	120	1,2,3-trimethyl benzene	4.481
1232	120	1-ethyl-4-methyl benzene	2.585
1252			0.550
1262			0.230
1303	120	1,3,5-trimethyl benzene	14.262
1323	142	decane	2.129
1353	134	(2-methylpropyl)benzene	0.245
1368	134	(1-methylpropyl)benzene	0.256
1383			0.066
1423	120	1,2,4-trimethyl benzene	5.955
1457	140	butyl cyclohexane	0.599
1478	118	1-ethenyl-2-methyl benzene	0.439
1493			0.275
1552	134	1-methyl-4-propyl benzene	0.991
1567	134	1-methyl-2-propyl benzene	0.161
1584	134	4-ethyl-1,2-dimethyl benzene	0.275
1606			0.125
1620	134	methyl benzencacetaldehyde	0.146
1635			0.104
1673	134	(1,1-dimethyl ethyl) benzene	0.550
1706	134	2-ethyl-1,4-dimethyl benzene	0.729
1770	156	undecane	2.241
1791	152	1-pentyl cyclohexene	0.098
1813		2-methyl-decahydro naphthalene	0.162
1843	134	1,2,3,5-tetramethyl benzene	0.355
1863	134	1,2,4,5-tetramethyl benzene	0.434
1888			0.379
1921			0.155
1942			0.091
2007	134	2-ethyl-1,4-dimethyl benzene	0.787
2034	170	2-methyl undecane	0.050
2084			0.113
2106			0.031
2120			0.022
2126			0.048

continued...

Table 6.2.9. Concluded.

Scan	M.W.	Compound	ppm^a	Scan	M.W	Compound	ppm^a
2153	168	1-methyl-2-pentyl cyclohexane	0.438				
2172			0.096				
2196			0.013				
2219	170	dodecane	1.643				
2277	184	2,6-dimethyl undecane	0.591				
2311			0.093				
2387			0.054				
2400			0.131				
2445			0.086				
2475			0.074				
2496			0.058				
2509			0.023				
2532			0.455				
2554			0.085				
2602			0.035				
2638	142	1-methyl naphthalene	0.825				
2643	142	2-methyl naphthalene	1.402				
2668			0.020				
2712		1,4-dihydro-1,4-methano naphthalene	0.901				
2726	142	methyl naphthalene	0.438				
2744			0.017				
2722			0.121				
2785			0.005				
2843			0.084				
2922			0.071				
2946			0.012				
2950			0.015				
2974			0.294				
3011			0.015				
3071			0.591				
3114	156	2,7-dimethyl naphthalene	0.192				
3175			0.193				
3181			0.141				
3262			0.024				
3267			0.037				
3320			0.067				
3472			0.036				

^{a}Approximate concentrations based on a volatile carbon content of 242 ppm.

Table 6.2.10. GP31 volatiles, 1981 March (82 ppm).

Scan	M.W.	Compound	ppm[a]
268			0.833
277			0.576
308			0.327
328			0.095
343	89	2-methyl-2-butanol	0.143
361	78	benzene	1.444
391	98	1,2-dimethyl cyclopentane	0.718
406	100	heptane	0.389
445	98	methyl cyclohexane	1.352
467			0.051
479	112	1,2,4-trimethyl cyclopentane	0.167
496	112	1,2,3-trimethyl cyclopentene	0.252
550	92	methyl benzene	2.968
580	112	1,4-dimethyl cyclohexane	0.603
639	112	1,3-dimethyl cyclohexane	0.589
661	114	octane	1.039
799	112	ethyl cyclohexane	2.061
839	126	1-ethyl-4-methyl cyclohexane	0.083
862	126	1,3,5-trimethyl cyclohexane	0.994
889	106	ethyl benzene	1.089
915	106	1,3-dimethyl benzene	7.966
935	126	1,1,2-trimethyl cyclohexane	0.180
955	126	1-ethyl-2-methyl cyclohexane	0.896
977	106	1,4-dimethyl benzene	5.810
999	128	nonane	1.830
1009			0.245
1040	124	1-methyl-octahydro pentalene	1.161
1062	120	(1-methylethyl)benzene	0.509
1074	126	propyl cyclohexane	0.537
1090	142	2,6-dimethyl octane	0.644
1110			0.974
1131			0.064
1147	120	propyl benzene	1.153
1162			0.023
1176	120	1-ethyl-3-methyl benzene	2.995
1197	120	1,2,3-trimethyl benzene	2.092
1210	126	1-ethyl-4-methyl cyclohexane	0.110
1227	120	1-ethyl-4-methyl benzene	1.141
1241	140	5-decene	0.449
1281	120	1,3,5-trimethyl benzene	5.570
1296	142	decane	1.829
1310			0.047
1316	134	(2-methylpropyl)benzene	0.041
1325	134	(1-methylpropyl)benzene	0.129
1337			0.062
1366	120	1,2,4-trimethyl benzene	2.999
1391			0.939
1405	118	1-ethenyl-2-methyl benzene	0.341
1417			0.194
1439			0.035
1465	138	decahydro naphthalene	0.661
1473	134	1-methyl-3-propyl benzene	0.134
1478			0.177
1484	134	4-ethyl-1,2-dimethyl benzene	0.312
1492	142	3,3,5-trimethyl heptane	0.126
1502	156	isooctane	0.274
1514	134	1-methyl-4-propyl benzene	0.097
1526			0.130
1538			0.046
1554			0.210
1583	134	4-ethyl-1,2-dimethyl benzene	0.476
1600	134	1-methyl-3-propyl benzene	0.044
1636	156	undecane	1.922
1666	152	2-methyl-decahydro naphthalene	0.084
1673			0.030
1695	134	1,2,3,5-tetramethyl benzene	0.160
1707	134	1,2,4,5-tetramethyl benzene	0.088
1726			0.144
1733	170	4-methyl undecane	0.116
1758			0.118
1781			0.104
1832	134	2-ethyl-1,4-dimethyl benzene	0.248
1839			0.078
1846			0.096
1878	170	2-methyl undecane	0.179
1904			0.093

continued...

Table 6.2.10. Concluded.

Scan	M.W.	Compound	ppm[a]
1930	166	1,6-dimethyl-decahydro naphthalene	0.071
1964			0.151
2023	170	dodecane	0.869
2079	184	2,6-dimethyl undecane	0.418
2102			0.054
2136			0.027
2142			0.009
2153			0.035
2170			0.007
2174			0.018
2186			0.068
2216			0.023
2221			0.011
2250			0.122
2262			0.016
2280			0.057
2315			0.481
2326			0.055
2340			0.007
2357			0.007
2377			0.032
2385			0.005
2389			0.002
2408			0.046
2426	184	tridecane	0.130
2460			0.038
2484			0.046
2498			0.060
2519			0.008
2523			0.010
2552			0.013
2569			0.053
2594			0.009
2629			0.031
2696			0.007
2714			0.007
2768			0.018
2772			0.023
2919			0.026
2931			0.003
3084			0.007
3203			0.007

[a] Approximate concentration based on a total volatile carbon content of 82 ppm.

Table 6.2.11. GP19 volatiles, 1981 May (25 ppm).

Scan	M.W.	Compound	ppm[a]
269	46	oxybis methane	0.117
281	56	2-methyl-1-propene	0.043
300	58	oxetane	2.939
312	74	2-methyl-2-propanol	0.528
363			0.815
394	84	methyl cyclopentane	0.027
412	88	2-methyl-2-butanol	0.192
445	78	benzene	4.231
499			0.085
523			0.127
541	100	3,3-dimethyl-2-butanone	0.059
568	98	methyl cyclohexane	0.109
639	94	dimethyl disulfide	0.085
713	92	methyl benzene	4.036
1284	106	ethyl benzene	0.526
1359	106	1,3-dimethyl benzene	2.977
1430			0.082
1486	106	1,4-dimethyl benzene	4.805
1533			0.036
1620	120	(1-methylethyl)benzene	0.226
1744			0.105
1776	120	1-ethyl-3-methyl benzene	0.317
1802	120	1,2,3-trimethyl benzene	0.193
1847	120	1-ethyl-4-methyl benzene	0.162
1904	120	1,3,5-trimethyl benzene	1.022
2022	120	1,2,4-trimethyl benzene	0.486
2124			0.016
2137	138	hexfluoro ethane	0.023
2142			0.013
2202			0.006
2207	134	diethyl benzene	0.008
2213			0.004
2230			0.010
2242			0.010
2292			0.006
2313			0.004
2318			0.019
3303			0.259
3482			0.011
3491			0.009
3502			0.007
3507			0.003
3511			0.002
3561			0.010

[a] Approximate concentration based on a total volatile carbon content of 25 ppm.

Table 6.2.12. GP19 volatiles, 1981 June (26 ppm).

Scan	M.W.	Compound	ppm[a]	Scan	M.W	Compound	ppm[a]
228			1.240				
241	84	methyl cyclopentane	0.144				
265	78	benzene	5.743				
422			0.221				
426			0.158				
433			0.039				
437	84	cyclopentanone	0.088				
519			2.836				
593			2.019				
780			0.307				
785			0.122				
789			0.282				
909			0.223				
913			0.187				
923			0.102				
1503	120	1-ethyl-3-methyl benzene	0.170				
1508			0.088				
1518	120	1-ethyl-4-methyl benzene	0.431				
1580			0.086				
1666			0.673				
1670			0.440				
1683	120	1,3,5-trimethyl benzene	0.189				
1811			0.105				
1817			0.110				
1822	120	1,2,4-trimethyl benzene	0.228				
1834			0.064				
1838	138	hexfluoro ethane	0.157				
2494			0.071				
2502			0.025				
2539			0.072				
2548			0.056				
3275			0.924				
3420			0.062				

[a] Approximate concentration based on a total volatile carbon content of 26 ppm.

Table 6.2.13. GP26 neutrals, 1981 May.

Scan	M.W.	Compound	Relative amount^a
246	78	sulfinylbis methane	24.290
357	120	1(1-propynyl) cyclohexane	15.230
372	156	undecane	18.733
426			5.961
436	134	1,2,3,5-tetramethyl benzene	21.130
451			5.288
467	166	2,3-dimethyl-decahydro napthalene ( )	7.452
478	128	napthalene	80.086
489	134	2-methyl-3-phenyl oxirane	20.261
496	170	dodecane	14.433
502	148	1,3-dimethyl-5-(1-methyl ethyl)benzene	7.880
517	134	ethyl benzaldehyde	12.064
537	168	cyclododecane	14.470
548			14.980
557	146	2,3-dihydro-4,7-dimethyl-IH-indene	8.560
563			6.871
576			30.951
604	146	2,3-dihydro-1,6-dimethyl-IH-indene	5.658
617	184	tridecane	54.243
627	142	2-methyl naphthalene	73.559
653	142	1-methyl naphthalene	54.906
691			21.611
701			5.576
716	198	2-methyl tridecane	16.142
727			11.601
737	198	2,5-dimethyl dodecane	19.236
760			9.207
766			6.078
779	198	tetradecane	100.000
801	156	1,7-dimethyl naphthalene	45.086
814	162	2,5-dimethyl-benzo-B-thiophene	7.047
826	156	1,2-dimethyl naphthalene	42.593
831	156	1,5-dimethyl naphthalene	31.089
838	162	ethyl-benzo-B-thiophene	9.029
861			43.033
876			11.043
883			47.846
891			12.075
897			9.955
909			22.818
935	168		7.737
941			7.021
952	212	pentadecane	93.373
970	170	2(1-methylethyl) napthalene	19.402
977			4.617
999			15.012
1009	170	1,6,7-trimethyl naphthalene	15.817
1016	170	2,3,6-trimethyl naphgthalene	16.474
1031			18.934
1043			29.343
1050	170	1,3,6-trimethyl naphthalene	25.329
1061	226	5-propyl tridecane	10.669
1074	170	trimethyl napthalene	18.878
1097			3.612
1110			17.628
1128	226	hexadecane	95.830
1138			13.254
1174			10.327
1185			8.182
1212			49.820
1224			20.087
1236			6.664
1248			10.887
1262	184	1-methyl-7(1-methylethyl)naphthalene	6.329
1302	240	heptadecane	78.321
1310	268	2,6,10,14-tetramethyl pentodacane	48.262
1322	180	9-methyl-9H-fluorene	8.356
1357			5.369
1375			21.616
1388			7.404
1401	184	dibenzothiophene	20.091
1419			6.842
1448	178	phenanthrene	13.861
1468	254	octadecane	60.012
1482	296	2,6,10,14-tetramethyl heptadecane	31.622
1538			8.946
1568	198	4-methyl dibenzothiophene	10.992
1616			7.165

continued...

Table 6.2.13. Concluded.

Scan	M.W.	Compound	Relative amount [a]	Scan	M.W	Compound	Relative amount [a]
1629	268	nonadecane	47.778	2294			4.881
1643	192	3-methyl phenanthrene	10.397	2345	338	tetracosane	5.896
1727	212	4,9-dimethyl-naphtho-2,3-B-thiophene	5.873	2394			2.477
1752			11.610	2399			1.395
1784	282	eicosane	24.377	2406			3.611
1850	206	2,5-dimethyl phenanthrene	5.907	2443			3.935
1933	296	heneicosane	17.041	2475	352	pentacosane	4.152
2076	310	docosane	10.299	2541			8.535
2108			4.918	2597			2.766
2142	324	2,3,5-trimethyl phenanthrene	6.060	2665			1.957
2153			0.559	2669			0.668
2158			1.527	2716			2.326
2178			4.717	2858			1.788
2214	324	tricosane	8.198	2907			1.978
2221			5.322	2979			2.945
2233			1.633	3123			5.558
2238	234	tetramethyl phenthrene	0.493	3213			4.304
2259			4.311	3320			1.777

[a] Relative amount of each component based on GC-MS peak areas; most abundant compound = 100.00.

Table 6.2.14. GP19 neutrals, 1981 May.

Scan	M.W.	Compound	Relative amount[a]
308	120	1-ethyl-3-methyl benzene	7.701
319	120	1-ethyl-2-methyl benzene	3.230
328	120	1,2,4-trimethyl benzene	22.409
348	120	1,3,5-trimethyl benzene	13.531
359	118	1-ethenyl-2-methyl benzene	4.623
370	134	1,4-diethyl benzene	11.951
389	134	1-(methylphenyl) ethanone	5.218
400	156	undecane	28.506
415	134	2-ethyl-1,4-dimethyl benzene	3.489
424	134	1-ethyl-3,5-dimethyl bezene	5.278
429	134	1,2,3,5-tetramethyl benzene	6.473
439	124	cyclopropyl cyclohexane	5.826
452			10.395
463	134	1,2,4,5-tetramethyl benzene	31.663
476	132	1,2,3,4-tetrahydro naphthalene	11.696
495			4.718
507	170	2-methyl undecane	100.000
516	146	2,3-dihydro-1,1-dimethyl-1H-indene	12.780
523	170	dodecane	18.385
528	148	2,4-dimethyl-1-(1-methylethyl) benzene	6.295
540	146	1,2,3,4-tetrahydro-2-methyl naphthalene	4.131
544			7.480
562	140	2-methylpropyl cyclohexane	13.060
575	158	2-propyl-1-heptanol	8.147
583	146	2,3-dihydro-4,7-dimethyl indene	8.644
590	184	2-methyl dodecane	6.882
603			33.260
629	146	2,3-dihydro-1,6-dimethyl indene	4.529
649	184	tridecane	71.446
658	142	2-methyl naphthalene	80.928
682	142	1-methyl naphthalene	65.002
697	160	2,3-dihydro-1,1,5-trimethyl indene	5.899
714			17.231
726	160	6-ethyl-1,2,3,4-tetrahydro naphthalene	3.650
733			3.173
742	198	2-methyl tridecane	10.442
753			7.124
763			22.803
781	154	1-1'-biphenyl	3.456
807	198	tetradecane	91.537
829	156	1,7-dimethyl naphthalene	42.355
854	156	1,8-dimethyl naphthalene	47.299
860	156	1,5-dimethyl naphthalene	31.011
885	156	1,3-dimethyl naphthalene	38.749
910			55.046
923	212	3-ethyl tridecane	6.176
934			7.813
940			2.717
960	154	1,2-dihydro acenaphthylene	7.607
964			5.255
981	212	pentadecane	99.425
996	170	2-(1-methylethyl) naphthalene	21.194
1032	170	1,6,7-trimethyl naphthalene	16.296
1041	170	2,3,6-trimethyl naphthalene	16.028
1068			37.935
1088	226	2-methyl pentadecane	7.193
1099			12.253
1136			11.534
1157	226	hexadecane	94.344
1164			15.511
1198	184	1-(1-1-dimethylethyl) naphthalene	2.327
1239			42.163
1250	224	decyl-cyclohexane	9.997
1261			4.384
1274	254	2-methyl hepladecane	6.427
1285	184	1-methyl-7-(1-methylethyl) naphthalene	2.174
1318			3.040
1331	240	heptadecane	74.671
1340	268	2,6,10,14-tetramethyl pentadecane	46.389
1347	180	9-methyl-9H-fluorene	3.183
1382			2.342
1399			10.898
1412			5.122
1425	222	1,1'-(1,4-butanediyl)bis-cyclohexane	8.081
1430	254	2-methyl heptadecane	5.129
1443			3.430

continued...

Table 6.2.14. Concluded.

Scan	M.W.	Compound	Relative amount[a]
1472	178	phenanthrene	5.475
1496	254	octadecone	56.907
1509	296	2,6,10,14-tetramethyl heptadecane	33.695
1559			4.667
1592			4.839
1605			2.933
1640			4.126
1655	268	nonadecane	37.943
1668	192	3-methyl phenanthrene	4.000
1749			2.060
1756			1.860
1780			2.084
1809	282	eicosane	22.111
1875	256	sulfur (S_8)	9.623
1919			2.844
1956			13.170
2099	296	heneicosane	9.611
2115	256	docosane	0.418
2127			1.068
2133			0.365
2146			1.740
2158			0.600
2172			0.427
2201			1.124
2236	324	tricosane	8.317
2258			1.160
2279			1.248
2314			1.562
2347			0.515
2368	338	tetracosane	3.544
2465			0.931
2496	352	pentacosane	1.010
2563			1.241
2807			0.590
2820			0.488
2878			0.353
2892			0.318
2969			0.355
2999			0.742
3020			0.578
3071			0.385

[a] Relative amount of each component based on GC-MS peak areas; most abundant compound = 100.00.

Table 6.2.15. GP26 acids, 1981 May.

Scan	M.W.	Compound	ppb
287	94	Phenol	483
307	116	C_8-acid	15
320	116	C_8-acid	91
342	108	C_1-Phenol	1080
364	108	C_1-Phenol	1575
391	122	C_2-Phenol	394
416	122	C_2-Phenol	558
439	122	C_2-Phenol	1812
454	122	C_2-Phenol	79
478	136	C_3-Phenol	1438
500	136	C_3-Phenol	147
513	136	C_3-Phenol	355
523	136	C_3-Phenol	41
542	136	C_3-Phenol	369
551	136	C_3-Phenol	456
562	136	C_3-Phenol	404
602	122	Benzoic acid	1006
614	136	C_3-Phenol	130
618	136	C_3-Phenol	74
625	136	C_3-Phenol	224
637	116	C_9-acid	31
643	150	C_4-Phenol	47
660	136	C_3-Phenol	118
690	134	Propenyl Phenol	446
701	150	C_4-Phenol	44
731	150	C_4-Phenol	515
763	148	Methylpropenyl phenol	441
777	136	C_1-Benzoic acid	106
789	148	C_2-Benzoic acid	149
804	148	Methylpropenyl phenol	100
870	148	Methylpropenyl phenol	253
879	150	C_2-Benzoic acid	33
899	150	C_2-Benzoic acid	92
937	162	C_2-Benzofuranone	175
949	150	C_2-Benzoic acid	67
959	164	C_3-Benzoic acid	115
970	150	C_2-Benzoic acid	28
993	164	C_3-Benzoic acid	42
1003	176	C_2-Benzofurandione	65
1010	170	Biphenylol	62
1036	144	Naphthalenol	164
1043	162	C_2-Benzofuranone	44
1055	150	C_4-Phenol	69
1086	190	Dichlorobenzoic acid	83
1112	162	C_2-Benzofuranone	72
1122	164	C_3-Benzoic acid	19

continued...

Table 6.2.15. Concluded.

Scan	M.W.	Compound	ppb
1195	158	C_1-Naphthalenol	80
1208	158	C_1-Naphthalenol	62
1244	158	C_1-Naphthalenol	165
1271	162	C_2-Dihydroindeneol	56
1296	164	C_3-Benzoic acid	18
1422	172	Naphthalenecarboxylic acid	72
1522	184	Phenylmethyl Phenol	27
1568	186	C_3-Naphthol	64
1596	184	Methoxyl Biphenyl	61

Table 6.2.16. GP19 acids, 1981 May.

Scan	M.W.	Compound	ppb
305	116	Pentanoic acid	44
314	94	Phenol	113
333	116	Hexanoic acid	296
364	108	C_1-Phenol	638
382	108	C_1-Phenol	523
389	144	C_2-Heptanol	22
413	122	C_2-Phenol	561
433	130	Heptanoic acid	482
438	122	C_2-Phenol	202
456	122	C_2-Phenol	1340
488	122	C_2-Phenol	403
496	136	C_3-Phenol	130
508	122	C_2-Phenol	262
521	136	C_3-Phenol	159
549	136	C_3-Phenol	390
564	136	C_3-Phenol	605
569	136	C_3-Phenol	447
577	144	Octanoic acid	317
597	136	C_3-Phenol	396
610	136	C_3-Phenol	337
616	136	C_3-Phenol	202
625	136	C_3-Phenol	209
659	136	C_3-Phenol	88
688	136	C_3-Phenol	384
747	136	C_1-Benzoic acid	41
773	150	C_2-Benzoic acid	189
807	148	C_4-Phenol	52
854	150	C_2-Benzoic acid	648
874	150	C_2-Benzoic acid	170
903	150	C_2-Benzoic acid	270
931	170	Cyclohexanebutanoic acid	59
945	150	C_2-Benzoic acid	127
968	150	C_2-Benzoic acid	183
973	150	C_2-Benzoic acid	32
988	164	C_3-Benzoic acid	54
1009	176	C_2-Benzofurandione	92
1040	164	C_3-Phenol	381
1057	164	C_3-Benzoic acid	52
1072	190	Dichlobenzoic acid	74
1082	164	C_3-Benzoic acid	70
1095	164	C_3-Benzoic acid	48
1112	164	C_3-Benzoic acid	39
1129	162	Hydroxypropenyl benzaldehyde	162
1143	190	Dichlobenzoic acid	59
1180	164	C_3-Benzoic acid	237

continued...

Table 6.2.16. Concluded.

Scan	M.W.	Compound	ppb
1210	162	Ethenyl benzenacetic acid	162
1264	178	C_4-Benzoic acid	97
1365	130	Isooctanol	337
1395	176	Tetrahydronaphthenecarboxylic acid	83
1405	172	Naphthalenecarboxylic acid	155
1477	172	Naphthalenecarboxylic acid	372
1539	184	Methoxybiphenyl	68
1556	184	Methoxybiphenyl	32
1560	186	C_3-Naphthol	30
1635	186	C_3-Naphthol	356
1742	182	Biphenylacarboxaldehyde	69
1765	182	Biphenylcarboxyaldehyde	44
2114	168	Dibenzofuran	24

Table 6.2.17. GP26 bases, 1981 May.

Scan	M.W.	Compound	ppb
266	107	Ethylpyridine	17
283	122	Methylphenyl hydrazine	12
291	93	Methylpyridine	9
356	107	Methylbenzamine	66
526	133	Tetrahydroquinoline	28
548	129	Isoquinoline	77
579	129	Quinoline	72
611	147	Tetrahydromethylisoquinoline	55
650	143	Methylquinoline	126
662	143	Methylquinoline	33
667	143	Methylisoquinoline	8
705	143	Methylisoquinoline	14
728	143	Methylquinoline	41
737	143	Methylquinoline	41
759	157	Dimethylquinoline	71
776	143	Methylquinoline	112
793	157	Dimethylquinoline	72
843	157	Dimethylquinoline	24
868	157	Dimethylquinoline	22
902	157	Ethylquinoline	57
937	157	Ethylquinoline	31
946	171	Propylquinoline	8
994	171	Trimethylquinoline	26
1009	171	Propylquinoline	12
1016	157	Ethyl isoquinoline	8
1060	171	Trimethylquinoline	25
1082	159	Trimethylindole	6
1142	169	Biphenylamine	47
1205	183	Methylphenylbenzamine	19
1235	172	Methylethylcinnoline	27
1248	172	Methylethylcinnoline	19
1504	179	Benzoquinoline/acridine/phenanthridine/fluorenimine	17
1597	179	Benzoquinoline/acridine/phenanthridine/fluorenimine	11
1617	163	Pentamethyl benzamine	5
1671	193	Methylbenzoquinoline	17

Table 6.2.18. GP19 bases, 1981 May.

Scan	M.W.	Compound	ppb
300	93	Benzamine	6
306	121	Trimethylpyridine	4
368	107	Methylbenzamine	46
372	107	Methylbenzamine	31
448	121	Methylethylpyridine	14
461	121	Ethylbenzamine	60
468	121	Methylethylpyridine	82
497	121	Methylethylpyridine	15
503	121	Methylethylpyridine	42
555	129	Isoquinoline	27
563	135	Ethylbenzenemethanamine	6
578	135	Ethylbenzenemethanamine	27
587	135	Ethylbenzenemethanamine	34
605	147	Dihydrodimethylindole	5
623	135	Ethylbenzemethanamine	22
635	135	Ethylbenzemethanamine	41
653	143	Methylquinoline	10
666	143	Methylquinoline	6
671	161	Trimethyldihydroindole	2
683	143	Methylquinoline	5
703	143	Methylquinoline	6
711	133	Tetrahydroquinoline	12
721	143	Methylquinoline	9
744	147	Tetrahydronaphthalenamine	3
777	131	Methylindole	8
802	157	Dimethylquinoline	6
867	157	Dimethylquinoline	9
887	175	Dimethylethylindole	5
896	145	Dimethylindole	5
928	175	Dimethylethylindole	3
941	145	Dimethylindole	3
1305	175	Dihydrodimethylethylindole	3
1638	180	Benzocinnoline	16
1675	181	Fluorenamine	5
1737	167	Carbazole	16

APPENDIX 6.3

Extractable constituents of combustion tube produced waters.

Table 6.3.1. Combustion tube water extractable aromatics, 1983 November.

Scan	M.W.	Compound	ppb
457	154	1,1'-Biphenyl	1.1
559	168	C_1-Biphenyl	0.85
579	168	C_1-Biphenyl	1.9
1035	178	Phenanthrene	3.0
1246	192	C_1-Phenanthrene	5.8
1363	212	C_2-Dibenzothiophene	5.7
1414	206	C_2-Phenanthrene	12
1423	206	C_2-Phenanthrene	4.2
1446	206	C_2-Phenanthrene	2.2
1511	226	C_3-Dibenzothiophene	6.1
1572	220	C_3-Phenanthrene	1.8
1585	220	C_3-Phenanthrene	16
1594	226	C_3-Dibenzothiophene	3.0
1607	220	C_3-Phenanthrene	3.3
1788	234	C_4-Phenanthrene	3.5

Table 6.3.2. Combustion tube water nitrogen components, 1983 November.

Scan	M.W.	Compound	ppb
306	129	Quinoline or Isoquinoline	1.5
431	143	C_1-Quinoline	0.48
433	147	C_1-Aminoindan	2.4
557	157	C_2-Quinoline	1.3
635	171	C_2-Aminonaphthalene	1.6
730	184	Diaminobiphenyl	1.0
745	184	Diaminobiphenyl	0.80
764	173	C_4-Indole	1.2
808	199	C_4-Aminonapthalene	0.41
849	199	C_4-Aminonapthalene	0.93
868	172	C_3-Cinnoline	0.74
901	213	C_5-Aminonaphthalene	1.1
944	171	C_3-Quinoline	1.6
966	173	C_4-Indole	0.57
994	199	C_5-Quinoline or C_4-Aminonaphthalene	1.5
1003	213	C_6-Quinoline	1.9
1006	198	C_1-Diaminobiphenyl	2.8
1038	227	C_6-Aminonaphthalene	1.2
1057	179	Benzo(h)quinoline	0.75
1086	213	C_6-Quinoline	8.2
1089	212	C_2-Diaminobiphenyl	8.2
1106	213	C_6-Quinoline	1.7
1110	179	Benzo(f)quinoline/Phenanthridine	1.1
1127	213	C_6-Quinoline	2.6
1159	227	C_7-Quinoline	14
1176	227	C_7-Quinoline	1.8
1192	227	C_7-Quinoline	1.1
1202	227	C_7-Quinoline	6.5
1210	227	C_7-Quinoline	1.2
1220	227	C_7-Quinoline	0.91
1233	209	C_2-Aminofluorene	4.7
1259	241	C_8-Quinoline	0.45
1276	241	C_8-Quinoline	1.0
1288	193	C_1-Benzoquinoline	0.61
1324	207	C_2-Benzoquinoline	0.77
1386	207	C_2-Benzoquinoline	23
1397	207	C_2-Benzoquinoline	4.0
1491	221	C_3-Benzoquinoline	2.7
1499	221	C_3-Benzoquinoline	1.1
1504	209	C_2-Aminofluorene	0.84
1520	221	C_3-Benzoquinoline	1.1
1525	209	C_2-Aminofluorene	2.1
1534	221	C_3-Benzoquinoline	6.4
1549	221	C_3-Benzoquinoline	3.3
1564	221	C_3-Benzoquinoline	6.9
1582	221	C_3-Benzoquinoline	14
1599	221	C_3-Benzoquinoline	1.2

continued...

Table 6.3.2. Concluded.

Scan	M.W.	Compound	ppb
1659	221	C_3-Benzoquinoline	2.1
1693	235	C_4-Benzoquinoline	1.8
1701	235	C_4-Benzoquinoline	0.62
1712	235	C_4-Benzoquinoline	1.5
1722	235	C_4-Benzoquinoline	0.53
1728	235	C_4-Benzoquinoline	0.98
1735	235	C_4-Benzoquinoline	0.70
1746	235	C_4-Benzoquinoline	2.3
1772	235	C_4-Benzoquinoline	1.6
1859	235	C_4-Benzoquinoline	0.38
2015	244	C_1-Naphthoquinoline	1.3
2032	244	C_1-Naphthoquinoline	0.71
2041	244	C_1-Naphthoquinoline	0.58
2053	244	C_1-Naphthoquinoline	2.2
2186	258	C_2-Naphthoquinoline	0.64
2193	258	C_2-Naphthoquinoline	1.6
2207	258	C_2-Naphthoquinoline	1.1
2222	258	C_2-Naphthoquinoline	0.84
2355	272	C_3-Naphthoquinoline	0.76
2365	272	C_3-Naphthoquinoline	0.60

APPENDIX 6.4

Extractable constituents of UMATAC wastewaters.

Table 6.4.1. UMATAC overhead vent water extractable aromatics, 1982 October.

Scan	M/W	Compound	ppb
668	130	Methylindene	18
680	130	Methylindene	35
735	128	Naphthalene	163
754	134	Benzothiophene	96
868	144	C_2-Indene	8
892	144	C_2-Indene	14
897	144	C_2-Indene	15
908	144	C_2-Indene	38
936	144	C_2-Indene	6
949	148	Methylbenzothiophene	37
957	144	C_2-Indene	13
965	142	2-Methylnaphthalene	354
982	148	Methylbenzothiophene	44
996	148	Methylbenzothiophene	127
999	142	1-Methylnaphthalene	259
1140	154	Biphenyl	20
1151	162	C_2-Benzothiophene	56
1164	156	C_2-Naphthalene	51
1167	162	C_2-Benzothiophene	40
1188	156	C_2-Naphthalene	239
1188	162	C_2-Benzothiophene	94
1201	162	C_2-Benzothiophene	118
1210	162	C_2-Benzothiophene	20
1215	156	C_2-Naphthalene	268
1217	162	C_2-Benzothiophene	30
1220	156	C_2-Naphthalene	174
1228	162	C_2-Benzothiophene	55
1249	156	C_2-Naphthalene	103
1254	156	C_2-Naphthalene	48
1277	156	C_2-Naphthalene	69
1329	154	Acenaphthene	38
1342	176	C_3-Benzothiophene	21
1343	168	C_1-Biphenyl	17
1344	170	C_3-Naphthalene	11
1359	168	C_1-Biphenyl	8
1361	176	C_3-Benzothiophene	34
1374	176	C_3-Benzothiophene	50
1383	176	C_3-Benzothiophene	44
1385	168	C_1-Biphenyl	8
1390	168	C_1-Biphenyl	6
1402	176	C_3-Benzothiophene	60
1413	170	C_3-Naphthalene	68
1436	176	C_3-Benzothiophene	46
1454	176	C_3-Benzothiophene	12
1508	166	Fluorene	37
1524	190	C_4-Benzothiophene	21

continued...

Table 6.4.1. Continued.

Scan	M/W	Compound	ppb
1530	184	C_4-Naphthalene	12
1530	168	C_1-Acenaphthene	16
1535	168	C_1-Acenaphthene	11
1538	182	C_2-Biphenyl	7
1542	168	C_1-Acenaphthene	32
1548	190	C_4-Benzothiophene	42
1554	182	C_2-Biphenyl	5
1555	168	C_1-Acenaphthene	17
1577	184	C_4-Naphthalene	9
1581	182	C_2-Biphenyl	14
1596	190	C_4-Benzothiophene	13
1598	184	C_4-Naphthalene	6
1602	182	C_2-Biphenyl	17
1621	190	C_4-Benzothiophene	11
1633	184	C_4-Naphthalene	27
1657	190	C_4-Benzothiophene	11
1668	184	C_4-Naphthalene	22
1685	190	C_4-Benzothiophene	12
1695	184	C_4-Naphthalene	21
1708	190	C_4-Benzothiophene	11
1711	180	C_1-Fluorene	27
1721	180	C_1-Fluorene	24
1733	182	C_2-Acenaphthene	10
1740	182	C_2-Acenaphthene	11
1750	182	C_2-Acenaphthene	7
1755	182	C_2-Acenaphthene	7
1760	182	C_2-Acenaphthene	10
1793	184	Dibenzothiophene	36
1802	182	C_2-Acenaphthene	8
1838	178	Phenanthrene	64
1853	178	Anthracene	8
1901	194	C_2-Fluorene	12
1910	194	C_2-Fluorene	10
1914	194	C_2-Fluorene	5
1922	194	C_2-Fluorene	11
1943	194	C_2-Fluorene	10
1955	198	C_1-Dibenzothiophene	20
1988	198	C_1-Dibenzothiophene	21
2021	192	C_1-Phenanthrene/ C_1-Anthracene	17
2022	198	C_1-Dibenzothiophene	15
2028	192	C_1-Phenanthrene/ C_1-Anthracene	21
2042	192	C_1-Phenanthrene/ C_1-Anthracene	4

continued...

Table 6.4.1. Continued.

Scan	M/W	Compound	ppb
2058	192	C_1-Phenanthrene/ C_1-Anthracene	21
2064	192	C_1-Phenanthrene/ C_1-Anthracene	15
2111	212	C_2-Dibenzothiophene	8
2134	212	C_2-Dibenzothiophene	6
2144	212	C_2-Dibenzothiophene	12
2180	212	C_2-Dibenzothiophene	25
2190	206	C_2-Phenanthrene/ C_2-Anthracene	5
2201	212	C_2-Dibenzothiophene	10
2204	206	C_2-Phenanthrene/ C_2-Anthracene	5
2229	206	C_2-Phenanthrene/ C_2-Anthracene	10
2230	212	C_2-Dibenzothiophene	4
2238	206	C_2-Phenanthrene/ C_2-Anthracene	10
2247	206	C_2-Phenanthrene/ C_2-Anthracene	7
2261	202	Fluoranthene	4
2262	206	C_2-Phenanthrene/ C_2-Anthracene	6
2282	226	C_3-Dibenzothiophene	8
2312	226	C_3-Dibenzothiophene	6
2328	226	C_3-Dibenzothiophene	6
2332	202	Pyrene	7
2346	226	C_3-Dibenzothiophene	5
2352	226	C_3-Dibenzothiophene	5
2361	220	C_3-Phenanthrene/ C_3-Anthracene	3
2374	226	C_3-Dibenzothiophene	6
2389	220	C_3-Phenanthrene C_3-Anthracene	6
2401	220	C_3-Phenanthrene/ C_3-Anthracene	8
2424	220	C_3-Phenanthrene/ C_3-Anthracene	5
2474	216	Benzo(a)fluorene	3
2500	216	Benzo(b)fluorene	3
2532	216	C_1-Pyrene	2
2542	216	C_1-Pyrene	1
2660	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	3
2689	234	Benzonaphthothiophene	0.7

continued...

Table 6.4.1. Concluded.

Scan	M/W	Compound	ppb
2702	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	2
2722	234	Benzonaphthothiophene	0.3
2736	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	4
2779	228	Benzo(a)anthracene	3
2791	228	Chrysene/Triphenylene	17
2824	248	C_1-Benzonaphthothiophene	0.3
2852	248	C_1-Benzonaphthothiophene	0.4
2884	248	C_1-Benzonaphthothiophene	0.5
2938	242	C_1-Benzo(a)anthracene/ C_1-Chrysene/C_1-Triphenylene	1.5
2949	242	C_1-Benzo(a)anthracene/ C_1-Chrysene/C_1-Triphenylene	0.7
2981	242	C_1-Benzo(a)anthracene/ C_1-Chrysene/C_1-Triphenylene	0.5
3147	252	Benzofluoranthene	20
3242	252	Benzo(a)pyrene	5
3268	252	Perylene	3
3566	276	Benzo(ghi)perylene	12
3617	278	Dibenzoanthracene	18

Table 6.4.2. UMATAC preheat vent water extractable aromatics, 1982 October.

Scan	M/W	Compound	ppb
718	128	Naphthalene	1.7
738	134	Benzothiophene	2.8
941	148	C_1-Benzothiophene	1.8
957	142	2-Methylnaphthalene	4.0
958	148	C_1-Benzothiophene	2.8
975	148	C_1-Benzothiophene	1.6
988	148	C_1-Benzothiophene	6.6
990	142	1-Methylnaphthalene	3.4
1136	154	Biphenyl	0.3
1148	162	C_2-Benzothiophene	2.9
1160	156	C_2-Naphthalene	0.6
1163	162	C_2-Benzothiophene	1.4
1180	162	C_2-Benzothiophene	4.7
1181	156	C_2-Naphthalene	2.2
1197	162	C_2-Benzothiophene	7.1
1209	156	C_2-Naphthalene	2.9
1212	162	C_2-Benzothiophene	1.2
1215	156	C_2-Naphthalene	3.0
1224	162	C_2-Benzothiophene	1.7
1245	156	C_2-Naphthalene	1.3
1252	156	C_2-Naphthalene	0.5
1262	170	C_3-Naphthalene	0.5
1274	156	C_2-Naphthalene	0.8
1329	154	Acenaphthene	0.8
1340	176	C_3-Benzothiophene	1.2
1356	176	C_3-Benzothiophene	2.2
1363	170	C_3-Naphthalene	0.5
1374	176	C_3-Benzothiophene	3.8
1374	170	C_3-Naphthalene	0.5
1402	176	C_3-Benzothiophene	4.0
1413	170	C_3-Naphthalene	1.5
1422	170	C_3-Naphthalene	1.4
1435	176	C_3-Benzothiophene	2.3
1450	176	C_3-Benzothiophene	7.2
1481	170	C_3-Naphthalene	1.4
1509	166	Fluorene	0.8
1517	190	C_4-Benzothiophene	1.1
1521	184	C_4-Naphthalene	4.1
1524	190	C_4-Benzothiophene	1.4
1530	168	C_1-Biphenyl	0.7
1533	184	C_4-Naphthalene	1.2
1543	168	C_1-Biphenyl	0.7
1547	190	C_4-Benzothiophene	3.2
1551	181	C_1-Fluorene	0.5
1555	168	C_1-Biphenyl	0.4
1596	190	C_4-Benzothiophene	1.8

continued...

Table 6.4.2. Continued.

Scan	M/W	Compound	ppb
1610	184	C_4-Naphthalene	2.5
1623	190	C_4-Benzothiophene	1.0
1634	184	C_4-Naphthalene	1.8
1640	184	C_4-Naphthalene	4.2
1658	184	C_4-Naphthalene	3.3
1658	190	C_4-Benzothiophene	1.1
1670	184	C_4-Naphthalene	1.6
1687	190	C_4-Benzothiophene	1.2
1708	190	C_4-Benzothiophene	1.0
1734	190	C_5-Naphthalene	2.7
1795	184	Dibenzothiophene	4.1
1840	178	Phenanthrene	2.0
1947	194	C_2-Fluorene	1.3
1959	198	C_1-Dibenzothiophene	5.4
2025	192	C_1-Phenanthrene	0.7
2033	192	C_1-Phenanthrene	1.6
2062	192	C_1-Phenanthrene	2.4
2068	192	C_1-Phenanthrene	1.6
2115	212	C_2-Dibenzothiophene	1.3
2182	212	C_2-Dibenzothiophene	4.7
2235	206	C_2-Phenanthrene	4.1
2243	206	C_2-Phenanthrene	2.1
2252	206	C_2-Phenanthrene	1.5
2287	226	C_3-Dibenzothiophene	1.5
2307	220	C_3-Phenanthrene	1.0
2334	226	C_3-Dibenzothiophene	2.6
2337	202	Pyrene	0.7
2359	226	C_3-Dibenzothiophene	1.8
2408	220	C_3-Phenanthrene	3.1
2514	220	C_3-Phenanthrene	2.1
2539	216	C_1-Pyrene	0.8
2697	234	Benzonaphthothiophene	1.0
2729	234	Benzonaphthothiophene	0.8
2786	228	Benzo(a)anthracene	0.7
2798	228	Chrysene/Triphenylene	4.1
2830	248	C_1-Benzonaphthothiophene	0.7
2858	248	C_1-Benzonaphthothiophene	1.0
2893	248	C_1-Benzonaphthothiophene	1.2
2920	248	C_1-Benzonaphthothiophene	0.6
2944	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benzo(a)anthracene	3.5
2956	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benzo(a)anthracene	1.7
2971	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benzo(a)anthracene	1.3
2978	262	C_2-Benzonaphthothiophene	0.6

continued...

Table 6.4.2. Concluded.

Scan	M/W	Compound	ppb
2988	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benzo(a)anthracene	1.0
3084	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benzo(a)anthracene	1.9
3109	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benzo(a)anthracene	2.3
3122	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benzo(a)anthracene	0.9
3138	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benzo(a)anthracene	2.1
3155	252	Benzofluoranthenes	0.9
3190	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benzo(a)anthracene	1.2
3235	252	Benzo(e)pyrene	1.0
3250	252	Benzo(a)pyrene	0.4
3277	252	Perylene	0.5

Table 6.4.3. UMATAC overhead vent water basic components, 1982 October.

Scan	M.W.	Compound	ppb
246	107	C_2-Pyridine or C_1-Aniline	3,400
263	107	C_2-Pyridine or C_1-Aniline	970
283	107	C_2-Pyridine or C_1-Aniline	98
293	121	C_3-Pyridine	720
327	107	C_2-Pyridine	110
333	94	C_1-Pyrimidine	29,000
337	107	C_2-Pyridine	530
356	121	C_3-Pyridine	5,200
366	107	C_2-Pyridine	1,600
376	121	C_3-Pyridine	2,300
388	121	C_3-Pyridine	2,800
400	121	C_3-Pyridine	660
406	121	C_3-Pyridine	290
411	121	C_3-Pyridine	1,300
423	121	C_3-Pyridine	200
459	107	C_2-Pyridine	460
468	121	C_3-Pyridine	1,400
482	108	C_2-Pyrimidine	5,500
494	108	C_2-Pyrimidine	920
499	121	C_3-Pyridine	2,800
504	135	C_4-Pyridine	4,100
512	135	C_4-Pyridine	730
526	121	C_3-Pyridine	520
532	121	C_3-Pyridine	320
534	108	C_2-Pyrimidine	20,000
545	135	C_4-Pyridine	2,400
547	121	C_3-Pyridine	1,500
552	135	C_4-Pyridine	1,300
561	135	C_4-Pyridine	320
577	135	C_4-Pyridine	170
586	135	C_4-Pyridine	1,200
606	135	C_4-Pyridine	210
621	135	C_4-Pyridine	940
625	135	C_4-Pyridine	700
630	135	C_4-Pyridine	430
654	135	C_4-Pyridine	6,500
658	121	C_3-Pyridine	1,100
670	135	C_4-Pyridine	1,800
680	121	C_3-Pyridine	2,100
684	122	C_3-Pyrimidine	920
727	133	Aminoindan	650
735	122	C_3-Pyrimidine	790
742	122	C_3-Pyrimidine	330
750	122	C_3-Pyrimidine	230
766	149	C_5-Pyridine	1,200
770	163	C_6-Pyridine	970
790	122	C_3-Pyrimidine	530
793	149	C_5-Pyridine	1.200

continued...

Table 6.4.3. Continued.

Scan	M.W.	Compound	ppb
810	133	Aminoindan	360
815	133	Aminoindan	710
818	149	C_5-Pyridine	2,500
826	135	C_4-Pyridine	1,500
844	129	Quinoline	660
868	147	C_1-Aminoindan	550
890	129	Isoquinoline	660
908	133	Aminoindan	350
936	147	C_1-Aminoindan	1,100
977	147	C_1-Aminoindan	1,600
993	143	C_1-Quinoline or C_1-Isoquinoline	1,700
994	147	C_1-Aminoindan	480
1007	161	C_2-Aminoindan	500
1030	143	C_1-Quinoline	420
1033	161	C_2-Aminoindan	420
1055	143	C_1-Quinoline	960
1072	147	C_1-Aminoindan	750
1097	161	C_2-Aminoindan	530
1128	143	C_1-Quinoline	880
1139	161	C_2-Aminoindan	890
1184	157	C_2-Quinoline or C_2-Isoquinoline	1,200
1188	163	C_6-Pyridine	780
1216	161	C_2-Aminoindan	1,500
1217	157	C_2-Quinoline	830
1259	157	C_2-Quinoline	4,200
1272	157	C_2-Quinoline	820
1291	161	C_2-Aminoindan	790
1336	175	C_3-Aminoindan	740
1384	171	C_3-Quinoline	530
1388	177	C_7-Pyridine	1,300
1405	171	C_3-Quinoline	350
1464	171	C_3-Quinoline	1,200
1469	171	C_3-Quinoline	1,500
1481	171	C_3-Quinoline	380
1538	191	C_8-Pyridine or C_7-Aniline	350
1554	184	Diaminobiphenyl	48
1574	185	C_4-Quinoline	93
1586	171	C_3-Quinoline	560
1599	191	C_8-Pyridine	360
1613	184	Diaminiobiphenyl	120
1614	185	C_4-Quinoline	99
1616	191	C_8-Pyridine	190
1624	169	Aminobiphenyl	170
1628	185	C_4-Quinoline	110
1667	185	C_4-Quinoline	150
1710	205	C_9-Pyridine	46
1721	185	C_4-Quinoline	140
1733	183	C_1-Aminobiphenyl	66

continued...

Table 6.4.3. Concluded.

Scan	M.W.	Compound	ppb
1763	205	C_9-Pyridine	50
1794	198	C_1-Diaminobiphenyl	12
1814	183	C_1-Aminobiphenyl	58
1856	199	C_5-Quinoline	4
1871	199	C_5-Quinoline	8
1874	179	Acridine	12
1879	183	C_1-Aminobiphenyl	42
1893	195	C_1-Aminofluorene	30
1911	179	Benzo(f)quinoline	5
1916	197	C_2-Aminobiphenyl	21
1922	197	C_2-Aminobiphenyl	19
1953	198	C_1-Diaminobiphenyl	10
2002	197	C_2-Aminobiphenyl	25

APPENDIX 6.5

Aromatic components of SHOP-produced oil.

Table 6.5.1. SHOP base oil aromatic components.

Scan	M/W	Compound	ppb
701	166	Fluorene	64
875	180	C_1-Fluorene	35
885	180	C_1-Fluorene	58
901	180	C_1-Fluorene	15
993	178	Phenanthrene/Anthracene	193
1022	194	C_2-Fluorene	1.5
1028	194	C_2-Fluorene	8.7
1052	194	C_2-Fluorene	21
1059	194	C_2-Fluorene	33
1072	194	C_2-Fluorene	29
1092	194	C_2-Fluorene	20
1117	194	C_2-Fluorene	11
1168	208	C_3-Fluorene	7.3
1170	192	C_1-Phenanthrene/ C_1-Anthracene	70
1176	192	C_1-Phenanthrene/ C_1-Anthracene	82
1196	208	C_3-Fluorene	6.1
1204	192	C_1-Phenanthrene/ C_1-Anthracene	124
1208	208	C_3-Fluorene	30
1211	192	C_1-Phenanthrene/ C_1-Anthracene	84
1219	208	C_3-Fluorene	5.0
1225	208	C_3-Fluorene	18
1229	208	C_3-Fluorene	14
1238	208	C_3-Fluorene	31
1245	208	C_3-Fluorene	20
1255	208	C_3-Fluorene	7.9
1263	208	C_3-Fluorene	16
1276	208	C_3-Fluorene	39
1289	208	C_3-Fluorene	40
1302	208	C_3-Fluorene	22
1307	206	C_2-Phenanthrene/ C_2-Anthracene	20
1311	208	C_3-Fluorene	8.1
1323	208	C_3-Fluorene	35
1331	206	C_2-Phenanthrene/ C_2-Anthracene	108
1342	208	C_3-Fluorene	9.6
1346	206	C_2-Phenanthrene/ C_2-Anthracene	63
1348	208	C_3-Fluorene	5.8
1352	206	C_2-Phenanthrene/ C_2-Anthracene	44
1373	206	C_2-Phenanthrene/ C_2-Anthracene	350

continued...

Table 6.5.1. Continued.

Scan	M/W	Compound	ppb
1376	226	C_3-Dibenzothiophene	24
1381	206	C_2-Phenanthrene/ C_2-Anthracene	154
1389	226	C_3-Dibenzothiophene	71
1390	206	C_2-Phenanthrene/ C_2-Anthracene	127
1398	206	C_2-Phenanthrene/ C_2-Anthracene	30
1404	206	C_2-Phenanthrene/ C_2-Anthracene	79
1413	226	C_3-Dibenzothiophene	5.3
1422	206	C_3-Dibenzothiophene	42
1423	226	C_3-Dibenzothiophene	140
1440	226	C_3-Dibenzothiophene	14.7
1444	206	C_2-Phenanthrene/ C_2-Anthracene	40
1449	208	C_3-Fluorene	28
1452	220	C_3-Phenanthrene/ C_3-Anthracene	8.4
1455	226	C_3-Dibenzothiophene	136
1469	226	C_3-Dibenzothiophene	98
1472	202	Pyrene/Fluoranthene	39
1475	220	C_3-Phenanthrene/ C_3-Anthracene	5.1
1481	220	C_3-Phenanthrene/ C_2-Anthracene	7.9
1487	226	C_3-Dibenzothiophene	83
1493	226	C_3-Dibenzothiophene	98
1502	220	C_3-Phenanthrene/ C_3-Anthracene	67
1511	240	C_4-Dibenzothiophene	17
1515	226	C_3-Dibenzothiophene	102
1526	226	C_3-Dibenzothiophene	9.7
1530	220	C_3-Phenanthrene/ C_3-Anthracene	92
1541	226	C_3-Dibenzothiophene	34
1543	220	C_3-Phenanthrene/ C_3-Anthracene	118
1551	226	C_3-Dibenzothiophene	47
1558	220	C_3-Phenanthrene/ C_3-Anthracene	32
1565	220	C_3-Phenanthrene/ C_3-Anthracene	73
1568	226	C_3-Dibenzothiophene	16
1577	220	C_3-Phenanthrene/ C_3-Anthracene	18
1582	220	C_3-Phenanthrene/ C_3-Anthracene	15

continued...

Table 6.5.1. Continued.

Scan	M/W	Compound	ppb
1584	240	C_4-Dibenzothiophene	31
1592	240	C_4-Dibenzothiophene	15
1593	220	C_3-Phenanthrene/ C_3-Anthracene	12
1603	220	C_3-Phenanthrene/ C_3-Anthracene	21
1607	240	C_4-Dibenzothiophene	11
1614	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	28
1620	240	C_4-Dibenzothiophene	8.4
1628	220	C_3-Phenanthrene/ C_3-Anthracene	17
1631	240	C_4-Dibenzothiophene	11
1642	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	22
1647	220	C_3-Phenanthrene/ C_3-Anthracene	98
1663	240	C_4-Dibenzothiophene	10
1672	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	30
1681	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	19
1685	240	C_4-Dibenzothiophene	12
1689	240	C_4-Dibenzothiophene	12
1707	240	C_4-Dibenzothiophene	20
1732	240	C_4-Dibenzothiophene	10
1733	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	3.2
1747	240	C_4-Dibenzothiophene	9.3
1774	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	9.5
1783	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	22
1802	230	C_2-Pyrene/C_3-Fluoranthene/ C_1-Benzofluorene	12
1809	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	11
1825	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	9.1
1834	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	7.8
1842	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	6.2
1863	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	19
1872	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	15

continued...

Table 6.5.1. Continued.

Scan	M/W	Compound	ppb
1880	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	3.0
1898	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	2.3
1929	228	Chrysene/Triphenylene	51
1932	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3.8
1941	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	4.2
1951	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5.0
1962	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3.9
1971	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	20
1994	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	4.4
2007	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	9.5
2019	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5.6
2026	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5.1
2045	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	9.1
2053	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	2.7
2076	242	C_1-Chrysene/C_1-Triphenylene	25
2078	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	3.4
2089	242	C_1-Chrysene/C_1-Triphenylene	10
2097	258	C_4-Pyrene/C_4-Fluoranthene/ C_4-Benzofluorene	2.5
2104	258	C_4-Pyrene/C_4-Fluoranthene/ C_4-Benzofluorene	9.9
2120	242	C_1-Chrysene/C_1-Triphenylene	8.2
2138	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	2.0
2148	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	8.8
2174	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	4.3
2182	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	3.7
2218	256	C_2-Chrysene/C_2-Triphenylene	13.7
2242	256	C_2-Chrysene/C_2-Triphenylene	14
2255	256	C_2-Chrysene/C_2-Triphenylene	5.8

continued...

Table 6.5.1. Concluded.

Scan	M/W	Compound	ppb
2264	256	C_2-Chrysene/C_2-Triphenylene	5.7
2271	256	C_2-Chrysene/C_2-Triphenylene	8.6
2283	256	C_2-Chrysene/C_2-Triphenylene	3.4
2289	252	Benzofluoranthene	4.6
2323	256	C_2-Chrysene/C_2-Triphenylene	13
2335	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	14
2355	270	C_3-Chrysene/C_3-Triphenylene	4.3
2367	252	Benzo(e)pyrene	18
2381	252	Benzo(a)pyrene	7.5
2388	270	C_3-Chrysene/C_3-Triphenylene	2.4
2397	270	C_3-Chrysene/C_3-Triphenylene	6.2
2411	252	Perylene	3.9
2466	270	C_3-Chrysene/C_3-Triphenylene	4.3
2497	270	C_3-Chrysene/C_3-Triphenylene	7.9
2505	266	C_1-Benzofluoranthene/Benzo(e)pyrene/Benzo(a)pyrene/Perylene	3.1
2525	284	C_4-Chrysene/C_4-Triphenylene	1.5
2540	266	C_1-Benzofluoranthene/Benzo(e)pyrene/Benzo(a)pyrene/Perylene	4.9
2549	266	C_1-Benzofluoranthene/Benzo(e)pyrene/Benzo(a)pyrene/Perylene	2.7
2620	284	C_4-Chrysene/C_4-Triphenylene	1.4
2626	280	C_2-Benzofluoranthene/Benzo(e)pyrene/Benzo(a)pyrene/Perylene	2.5
2630	280	C_2-Benzofluoranthene/Benzo(e)pyrene/Benzo(a)pyrene/Perylene	1.4
2653	284	C_4-Chrysene/C_4-Triphenylene	3.0
2671	280	C_2-Benzofluoranthene/Benzo(e)pyrene/Benzo(a)pyrene/Perylene	2.8
2681	280	C_2-Benzofluoranthene/Benzo(e)pyrene/Benzo(a)pyrene/Perylene	1.1

Table 6.5.2. SHOP P1 oil aromatic components, 1983 January.

Scan	MW	Compound	ppm
1468	166	Fluorene	61
1669	180	C_1-Fluorene	34
1678	180	C_1-Fluorene	61
1696	180	C_1-Fluorene	14
1794	178	Phenanthrene/Anthracene	229
1859	194	C_2-Fluorene	16
1867	194	C_2-Fluorene	31
1879	194	C_2-Fluorene	27
1900	194	C_2-Fluorene	20
1926	194	C_2-Fluorene	8
1978	192	C_1-Phenanthrene/C_1-Anthracene	83
1986	192	C_1-Phenanthrene/C_1-Anthracene	98
2014	192	C_1-Phenanthrene/C_1-Anthracene	156
2022	192	C_1-Phenanthrene/C_1-Anthracene	103
2052	208	C_3-Fluorene	24
2068	208	C_3-Fluorene	20
2089	208	C_3-Fluorene	27
2011	192	C_1-Phenanthrene/C_1-Anthracene	156
2117	208	C_3-Fluorene	17
2122	206	C_2-Phenanthrene/C_2-Anthracene	19
2136	208	C_2-Phenanthrene/C_2-Anthracene	34
2146	206	C_2-Phenanthrene/C_2-Anthracene	66
2151	206	C_2-Phenanthrene/C_2-Anthracene	37
2162	206	C_2-Phenanthrene/C_2-Anthracene	64
2187	206	C_2-Phenanthrene/C_2-Anthracene	334
2191	226	C_3-Dibenzothiophene	21
2196	206	C_2-Phenanthrene/C_2-Anthracene	164
2204	206	C_2-Phenanthrene/C_2-Anthracene	122
2204	226	C_3-Dibenzothiophene	66
2219	206	C_2-Phenanthrene/C_2-Anthracene	80
2239	226	C_2-Dibenzothiophene	144
2257	226	C_2-Dibenzothiophene	12
2260	206	C_2-Phenanthrene/C_2-Anthracene	45
2271	226	C_2-Dibenzothiophene	187
2285	226	C_2-Dibenzothiophene	119
2288	202	Pyrene/Fluoranthrene	56
2304	226	C_2-Dibenzothiophene	123
2310	226	C_2-Dibenzothiophene	137
2319	220	C_3-Phenanthrene/C_3-Anthracene	98
2328	240	C_3-Dibenzothiophene	18
2332	226	C_2-Dibenzothiophene	149
2343	226	C_2-Dibenzothiophene	15
2347	220	C_3-Phenanthrene/C_3-Anthracene	132
2348	240	C_3-Dibenzothiophene	31
2358	226	C_2-Dibenzothiophene	45
2360	220	C_3-Phenanthrene/C_3-Anthracene	175

continued...

Table 6.5.2. Continued.

Scan	MW	Compound	ppm
2368	240	C_3-Dibenzothiophene	25
2386	226	C_2-Dibenzothiophene	22
2392	226	C_2-Dibenzothiophene	11
2402	240	C_3-Dibenzothiophene	39
2410	240	C_3-Dibenzothiophene	15
2412	220	C_3-Phenanthrene/C_3-Anthracene	18
2432	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	51
2439	240	C_3-Dibenzothiophene	13
2449	240	C_3-Dibenzothiophene	15
2459	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	38
2465	220	C_3-Phenanthrene/C_3-Anthracene	166
2482	240	C_3-Dibenzothiophene	17
2490	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	57
2504	240	C_3-Dibenzothiophene	28
2527	240	C_3-Dibenzothiophene	31
2552	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	6
2594	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	16
2603	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	45
2621	230	C_2-Pyrene/C_3-Fluoranthene/ C_1-Benzofluorene	25
2628	230	C_2-Pyrene/C_3-Fluoranthene/ C_1-Benzofluorene	21
2644	230	C_1-Pyrene/C_3-Fluoranthene/ C_1-Benzofluorene	19
2654	230	C_1-Pyrene/C_3-Fluoranthene/ C_1-Benzofluorene	17
2682	230	C_1-Pyrene/C_3-Fluoranthene/ C_1-Benzofluorene	39
2692	230	C_1-Pyrene/C_3-Fluoranthene/ C_1-Benzofluorene	32
2750	228	Chrysene/Triphenylene	102
2792	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	41
2828	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	21
2806	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	30
2899	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benz(a)anthracene	62
2909	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benz(a)anthracene	26

continued...

Table 6.5.2. Concluded.

Scan	MW	Compound	ppm
2925	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benz(a)anthracene	19
2941	242	C_1-Chrysene/C_1-Triphenylene/ C_1-Benz(a)anthracene	19
3038	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	23
3052	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	5
2063	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	19
2076	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	8
2086	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	9
2092	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	13
3105	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	5
3111	252	Benzofluoranthene	7
3144	256	C_2-Chrysene/C_2-Triphenylene/ C_2-Benz(a)anthracene	20
3171	270	C_3-Chrysene/C_3-Triphenylene/ C_3-Benz(a)anthracene	3
3176	270	C_3-Chrysene/C_3-Triphenylene/ C_3-Benz(a)anthracene	4
3190	252	Benzo(e)pyrene	17
3208	252	Benzo(a)pyrene	1.9
3211	270	C_3-Chrysene/C_3-Triphenylene/ C_3-Benz(a)anthracene	6
3218	270	C_3-Chrysene/C_3-Triphenylene/ C_3-Benz(a)anthracene	9
3241	270	C_3-Chrysene/C_3-Triphenylene/ C_3-Benz(a)anthracene	4
3289	270	C_3-Chrysene/C_3-Triphenylene/ C_3-Benz(a)anthracene	5
3318	270	C_3-Chrysene/C_3-Triphenylene/ C_3-Benz(a)anthracene	11
3320	266	C_1-Benzopyrene/C_1-Benzofluoranthene	2
3327	266	C_1-Benzopyrene/C_1-Benzofluoranthene	4
3362	266	C_1-Benzopyrene/C_1-Benzofluoranthene	6
3371	266	C_1-Benzopyrene/C_1-Benzofluoranthene	4

Table 6.5.3. SHOP P1 oil aromatic components, 1983 May.

Scan	M.W.	Compound	ppm
700	166	Fluorene	47
875	180	C_1-Fluorene	23
885	180	C_1-Fluorene	41
901	180	C_1-Fluorene	9
993	178	Phenanthrene	15
1028	194	C_2-Fluorene	6
1052	194	C_2-Fluorene	12
1060	194	C_2-Fluorene	21
1072	194	C_2-Fluorene	17
1092	194	C_2-Fluorene	12
1117	194	C_2-Fluorene	5
1169	192	C_1-Phenanthrene/C_1-Anthracene	57
1176	192	C_1-Phenanthrene/C_1-Anthracene	66
1204	192	C_1-Phenanthrene/C_1-Anthracene	9
1208	208	C_3-Fluorene	12
1211	192	C_1-Phenanthrene/C_1-Anthracene	6
1227	208	C_1-Phenanthrene/C_1-Anthracene	12
1239	208	C_1-Phenanthrene/C_1-Anthracene	13
1245	208	C_1-Phenanthrene/C_1-Anthracene	9
1276	208	C_1-Phenanthrene/C_1-Anthracene	16
1289	208	C_1-Phenanthrene/C_1-Anthracene	20
1302	208	C_1-Phenanthrene/C_1-Anthracene	10
1308	206	C_2-Phenanthrene/C_2-Anthracene	11
1323	208	C_3-Fluorene	22
1332	206	C_2-Phenanthrene/C_2-Anthracene	61
1342	208	C_3-Fluorene	6
1347	206	C_2-Phenanthrene/C_2-Anthracene	35
1352	206	C_2-Phenanthrene/C_2-Anthracene	26
1373	206	C_2-Phenanthrene/C_2-Anthracene	197
1376	226	C_3-Dibenzothiophene	11
1381	206	C_2-Phenanthrene/C_2-Anthracene	90
1389	206	C_2-Phenanthrene/C_2-Anthracene	75
1398	206	C_2-Phenanthrene/C_2-Anthracene	18
1404	206	C_2-Phenanthrene/C_2-Anthracene	46
1413	226	C_2-Dibenzothiophene	
1421	206	C_2-Phenanthrene/C_2-Anthracene	25
1423	226	C_3-Dibenzothiophene	65
1444	206	C_2-Phenanthrene/C_2-Anthracene	26
1449	208	C_3-Fluorene	18
1452	220	C_3-Phenanthrene/C_3-Anthracene	6
1452	226	C_3-Dibenzothiophene	64
1468	226	C_3-Dibenzothiophene	46
1472	202	Pyrene	27
1473	206	C_2-Phenanthrene/C_2-Anthracene	8

continued...

Table 6.5.3. Continued.

Scan	M.W.	Compound	ppm
1487	226	C_3-Dibenzothiophene	42
1493	226	C_3-Dibenzothiophene	52
1502	220	C_3-Phenanthrene/C_3-Anthracene	38
1510	240	C_4-Dibenzothiophene	6
1514	226	C_3-Dibenzothiophene	58
1529	220	C_3-Phenanthrene/C_3-Anthracene	50
1540	226	C_3-Dibenzothiophene	19
1543	220	C_3-Phenanthrene/C_3-Anthracene	65
1549	226	C_3-Dibenzothiophene	25
1557	220	C_3-Phenanthrene/C_3-Anthracene	17
1564	220	C_3-Phenanthrene/C_3-Anthracene	42
1568	226	C_3-Dibenzothiophene	10
1576	220	C_3-Phenanthrene/C_3-Anthracene	8
1581	220	C_3-Phenanthrene/C_3-Anthracene	10
1583	240	C_4-Dibenzothiophene	12
1592	220	C_3-Phenanthrene/C_3-Anthracene	7
1602	220	C_3-Phenanthrene/C_3-Anthracene	13
1606	240	C_4-Dibenzothiophene	4
1613	216	C_1-Pyrene/C_1-Fluoranthrene/ Benzofluorene	24
1620	240	C_4-Dibenzothiophene	3
1627	220	C_3-Phenanthrene/C_3-Anthracene	11

Scan	M.W.	Compound	ppm
1639	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	17
1647	220	C_3-Phenanthrene/C_3-Anthracene	66
1662	240	C_4-Dibenzothiophene	5
1671	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	25
1680	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	18
1687	240	C_4-Dibenzothiophene	12
1746	240	C_4-Dibenzothiophene	7
1773	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	7
1782	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	19
1801	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	11
1824	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	9
1824	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	7
1832	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	6

continued...

Table 6.5.3. Continued.

Scan	M.W.	Compound	ppm
1841	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	5
1862	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	16
1871	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	13
1879	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	4
1897	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	2
1922	240	C_4-Dibenzothiophene	
1929	228	Chrysene/Triphenylene	42
1931	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3
1940	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3
1950	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3
1962	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	4
1971	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	15
1993	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	4
2007	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	8
2020	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5
2026	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5
2045	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	7
2053	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3
2062	244	C_3-Pyrene/C_3-Fluoranthene	4
2076	242	C_1-Chrysene/C_1-Triphenylene	25
2088	242	C_1-Chrysene/C_1-Triphenylene	10
2103	242	C_1-Chrysene/C_1-Triphenylene	7
2107	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	7
2120	242	C_1-Chrysene/C_1-Triphenylene	8
2148	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	4
2175	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	2

continued...

Table 6.5.3. Concluded.

Scan	M.W.	Compound	ppm
2183	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	2
2218	256	C_2-Chrysene/C_2-Triphenylene	9
2242	256	C_2-Chrysene/C_2-Triphenylene	8
2255	256	C_2-Chrysene/C_2-Triphenylene	4
2265	256	C_2-Chrysene/C_2-Triphenylene	3
2271	256	C_2-Chrysene/C_2-Triphenylene	6
2284	256	C_2-Chrysene/C_2-Triphenylene	2
2289	252	Benzofluoranthene	3
2324	256	C_2-Chrysene/C_2-Triphenylene	8
2336	258	C_4-Pyrene/C_4-Fluoranthene/ C_3-Benzofluorene	7
2357	270	C_3-Chrysene/C_3-Triphenylene	2
2368	252	Benzo(e)pyrene	8
2384	252	Benzo(a)pyrene	1.5
2390	270	C_3-Chrysene/C_3-Triphenylene	3
2397	270	C_3-Chrysene/C_3-Triphenylene	4
2419	270	C_3-Chrysene/C_3-Triphenylene	2
2437	266	C_1-Benzofluoranthene/C_1-Benzopyrene	1.6
2468	270	C_3-Chrysene/C_3-Triphenylene	2
2498	270	C_3-Chrysene/C_3-Triphenylene	4
2499	266	C_1-Benzofluoranthene/C_1-Benzopyrene	1.4
2505	266	C_1-Benzofluoranthene/C_1-Benzopyrene	2
2527	284	C_4-Chrysene/C_4-Triphenylene	1
2541	266	C_1-Benzofluoranthene/ C_1-Benzopyrene	3
2550	266	C_1-Benzofluoranthene/ C_1-Benzopyrene	2
2628	280	C_2-Benzofluoranthene/ C_2-Benzopyrene	1.2
2633	280	C_2-Benzofluoranthene/ C_2-Benzopyrene	1.0
2655	284	C_4-Chrysene/C_4-Triphenylene	2
2673	280	C_2-Benzofluoranthene/ C_2-Benzopyrene	1.6
2680	280	C_2-Benzofluoranthene/ C_2-Benzopyrene	0.7
2777	276	Benzo(ghi)perylene	0.9

Table 6.5.4. SHOP P3 oil aromatic components, 1983 February.

Scan	M.W.	Compound	ppm
698	166	Fluorene	86
873	180	C_1-Fluorene	56
882	180	C_1-Fluorene	56
898	180	C_1-Fluorene	14
990	178	Phenanthrene	196
1026	194	C_2-Fluorene	9
1050	194	C_2-Fluorene	24
1058	194	C_2-Fluorene	21
1062	194	C_2-Fluorene	14
1069	194	C_2-Fluorene	25
1089	194	C_2-Fluorene	19
1114	194	C_2-Fluorene	8
1166	192	C_1-Phenanthrene/C_1-Anthracene	72
1173	192	C_1-Phenanthrene/C_1-Anthracene	80
1191	192	C_1-Phenanthrene/C_1-Anthracene	15
1200	192	C_1-Phenanthrene/C_1-Anthracene	139
1205	208	C_3-Fluorene	9
1208	192	C_1-Phenanthrene/C_1-Anthracene	89
1226	208	C_3-Fluorene	12
1236	208	C_3-Fluorene	9
1242	208	C_3-Fluorene	7
1261	208	C_3-Fluorene	5
1273	208	C_3-Fluorene	13
1286	208	C_3-Fluorene	15
1299	208	C_3-Fluorene	8
1305	206	C_2-Phenanthrene/C_2-Anthracene	7
1319	208	C_3-Fluorene	13
1329	206	C_2-Phenanthrene/C_2-Anthracene	39
1340	208	C_3-Fluorene	4
1344	206	C_2-Phenanthrene/C_2-Anthracene	25
1350	206	C_2-Phenanthrene/C_2-Anthracene	20
1368	208	C_3-Fluorene	4
1370	206	C_2-Phenanthrene/C_2-Anthracene	119
1373	225	C_3-Dibenzothiophene	25
1395	206	C_2-Phenanthrene/C_2-Anthracene	10
1401	206	C_2-Phenanthrene/C_2-Anthracene	28
1419	206	C_2-Phenanthrene/C_2-Anthracene	16
1420	226	C_2-Dibenzothiophene	48
1438	226	C_3-Dibenzothiophene	6
1441	206	C_2-Phenanthrene/C_2-Anthracene	16
1447	208	C_3-Fluorene	12
1449	220	C_3-Phenanthrene/C_3-Anthracene	5
1452	226	C_3-Dibenzothiophene	51
1465	226	C_3-Dibenzothiophene	37

continued...

Table 6.5.4. Continued.

Scan	M.W.	Compound	ppm
1466	208	C_3-Fluorene	4
1470	202	Pyrene/Fluoranthene	15
1471	220	C_3-Phenanthrene/C_3-Anthracene	4
1478	220	C_3-Phenanthrene/C_3-Anthracene	3
1484	226	C_3-Dibenzothiophene	33
1490	226	C_3-Dibenzothiophene	38
1500	220	C_3-Phenanthrene	27
1507	240	C_4-Dibenzothiophene	6
1512	226	C_3-Dibenzothiophene	42
1523	226	C_3-Dibenzothiophene	5
1527	240	C_4-Dibenzothiophene	9
1539	220	C_3-Phenanthrene/C_3-Anthracene	48
1547	226	C_3-Benzothiophene	14
1555	220	C_3-Phenanthrene/C_3-Anthracene	13
1562	220	C_3-Phenanthrene/C_3-Anthracene	29
1565	226	C_3-Benzothiophene	6
1574	220	C_3-Phenanthrene/C_3-Anthracene	6
1579	220	C_3-Phenanthrene/C_3-Anthracene	7
1580	240	C_4-Dibenzothiophene	13
1588	240	C_4-Dibenzothiophene	5
1591	220	C_3-Phenanthrene/C_3-Anthracene	5
1600	220	C_3-Phenanthrene/C_3-Anthracene	5
1604	240	C_4-Dibenzothiophene	4
1611	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	16
1625	220	C_3-Phenanthrene/C_3-Anthracene	8
1628	240	C_4-Dibenzothiophene	5
1638	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	11
1644	220	C_3-Phenanthrene/C_3-Anthracene	47
1660	240	C_4-Dibenzothiophene	5
1669	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	17
1679	216	C_1-Pyrene/C_1-Fluoranthene/ Benzofluorene	12
1682	240	C_4-Dibenzothiophene	5
1686	240	C_4-Dibenzothiophene	6
1705	240	C_4-Dibenzothiophene	9
1730	240	C_4-Dibenzothiophene	4
1745	240	C_4-Dibenzothiophene	5
1771	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	5
1780	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	16

continued...

Table 6.5.4. Continued.

Scan	M.W.	Compound	ppm
1799	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	8
1807	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	6
1821	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	5
1831	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	5
1840	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	4
1860	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	16
1870	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	10
1878	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	2
1896	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	2
1927	228	Chrysene/Triphenylene	34
1930	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3
1939	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3
1949	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3
1961	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	4
1969	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	19
1992	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	7
2005	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	8
2007	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	4
2018	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	7
2024	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5
2044	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	6
2061	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	4

continued...

Table 6.5.4. Concluded.

Scan	M.W.	Compound	ppm
2075	242	C_1-Chrysene/C_1-Triphenylene	21
2087	242	C_1-Chrysene/C_1-Triphenylene	10
2102	242	C_1-Chrysene/C_1-Triphenylene	6
2118	242	C_1-Chrysene/C_1-Triphenylene	7
2216	256	C_2-Chrysene/C_2-Triphenylene	9
2240	256	C_2-Chrysene/C_2-Triphenylene	9
2253	256	C_2-Chrysene/C_2-Triphenylene	3
2269	256	C_2-Chrysene/C_2-Triphenylene	6
2282	256	C_2-Chrysene/C_2-Triphenylene	2
2288	252	Benzofluoranthene	4.1
2322	256	C_2-Chrysene/C_2-Triphenylene	9
2354	270	C_3-Chrysene/C_3-Triphenylene	2
2367	252	Benzo(e)pyrene	8.8
2380	270	C_3-Chrysene/C_3-Triphenylene	2
2383	252	Benzo(a)pyrene	1.6
2387	270	C_3-Chrysene/C_3-Triphenylene	2
2396	270	C_3-Chrysene/C_3-Triphenylene	4
2434	266	C_1-Benzofluoranthene/ C_1-Benzopyrene	3
2465	270	C_3-Chrysene/C_3-Triphenylene	3
2496	270	C_3-Chrysene/C_3-Triphenylene	6
2503	266	C_1-Benzofluoranthene/ C_1-Benzopyrene	3
2538	266	C_1-Benzofluoranthene/ C_1-Benzopyrene	5
2547	266	C_1-Benzofluoranthene C_1-Benzopyrene	3

Table 6.5.5. SHOP P3 oil aromatic components, 1983 May.

Scan	M/W	Compound	ppb
704	166	Fluorene	67
876	180	C_1-Fluorene	32
886	180	C_1-Fluorene	60
990	180	C_1-Fluorene	13
993	178	Phenanthrene	247
1028	194	C_2-Fluorene	8
1052	194	C_2-Fluorene	16
1059	194	C_2-Fluorene	16
1064	194	C_2-Fluorene	10
1072	194	C_2-Fluorene	25
1092	194	C_2-Fluorene	17
1116	194	C_2-Fluorene	7
1168	192	C_1-Phenanthrene/C_1-Anthracene	82
1175	192	C_1-Phenanthrene/C_1-Anthracene	94
1203	192	C_1-Phenanthrene/C_1-Anthracene	148
1207	208	C_3-Fluorene	16
1210	192	C_1-Phenanthrene/C_1-Anthracene	99
1225	208	C_3-Fluorene	16
1237	208	C_3-Fluorene	15
1243	208	C_3-Fluorene	11
1253	208	C_3-Fluorene	5
1262	208	C_3-Fluorene	6
1275	208	C_3-Fluorene	21
1288	208	C_3-Fluorene	25
1301	208	C_3-Fluorene	13
1306	206	C_2-Phenanthrene/C_2-Anthracene	14
1321	208	C_3-Fluorene	28
1330	206	C_2-Phenanthrene/C_2-Anthracene	79
1340	208	C_3-Fluorene	7
1345	206	C_2-Phenanthrene/C_2-Anthracene	47
1350	206	C_2-Phenanthrene/C_2-Anthracene	33
1372	206	C_2-Phenanthrene/C_2-Anthracene	254
1375	226	C_3-Dibenzothiophene	13
1379	206	C_2-Phenanthrene/C_2-Anthracene	119
1387	226	C_3-Dibenzothiophene	38
1396	206	C_2-Phenanthrene/C_2-Anthracene	26
1402	206	C_2-Phenanthrene/C_2-Anthracene	56
1421	226	C_3-Dibenzothiophene	85
1439	226	C_3-Dibenzothiophene	8
1442	206	C_2-Phenanthrene/C_2-Anthracene	33
1453	226	C_3-Dibenzothiophene	81
1466	226	C_3-Dibenzothiophene	58
1470	202	Pyrene	36
1472	206	C_2-Phenanthrene/C_2-Anthracene	36
1479	220	C_3-Phenanthrene/C_3-Anthracene	8

continued...

Table 6.5.5. Continued.

Scan	M/W	Compound	ppb
1485	226	C_3-Dibenzothiophene	55
1491	226	C_3-Dibenzothiophene	60
1500	220	C_3-Phenanthrene/C_3-Anthracene	46
1508	240	C_4-Dibenzothiophene	7
1513	226	C_3-Dibenzothiophene	71
1523	226	C_3-Dibenzothiophene	6
1529	240	C_4-Dibenzothiophene	12
1531	220	C_3-Phenanthrene/C_3-Anthracene	65
1538	226	C_3-Dibenzothiophene	26
1541	220	C_3-Phenanthrene/C_3-Anthracene	84
1549	226	C_3-Dibenzothiophene	33
1556	220	C_3-Phenanthrene/C_3-Anthracene	21
1560	240	C_4-Dibenzothiophene	6
1562	220	C_3-Phenanthrene/C_3-Anthracene	55
1566	226	C_3-Dibenzothiophene	13
1572	226	C_3-Dibenzothiophene	5
1574	220	C_3-Phenanthrene/C_3-Anthracene	12
1580	220	C_3-Phenanthrene/C_3-Anthracene	12
1589	240	C_4-Dibenzothiophene	6
1591	220	C_3-Phenanthrene/C_3-Anthracene	12
1600	220	C_3-Phenanthrene/C_3-Anthracene	17
1605	220	C_3-Phenanthrene/C_3-Anthracene	5
1610	220	C_3-Phenanthrene/C_3-Anthracene	11
1612	216	C_1-Pyrene/C_1-Fluoranthene	31
1618	240	C_4-Dibenzothiophene	4
1626	220	C_3-Phenanthrene/C_3-Anthracene	13
1638	216	C_1-Pyrene/C_1-Fluoranthene	22
1660	240	C_4-Dibenzothiophene	6
1669	216	C_1-Pyrene/C_1-Fluoranthene	32
1679	216	C_1-Pyrene/C_1-Fluoranthene	20
1682	240	C_4-Dibenzothiophene	14
1698	240	C_4-Dibenzothiophene	2
1705	240	C_4-Dibenzothiophene	11
1731	240	C_4-Dibenzothiophene	10
1745	240	C_4-Dibenzothiophene	8
1771	230	C_2-Pyrene/C_2-Fluoranthene	10
1780	230	C_2-Pyrene/C_2-Fluoranthene	24
1799	230	C_2-Pyrene/C_2-Fluoranthene	13
1807	230	C_2-Pyrene/C_2-Fluoranthene	11
1822	230	C_2-Pyrene/C_2-Fluoranthene	10
1831	230	C_2-Pyrene/C_2-Fluoranthene	8
1839	230	C_2-Pyrene/C_2-Fluoranthene	7
1859	230	C_2-Pyrene/C_2-Fluoranthene	21
1869	230	C_2-Pyrene/C_2-Fluoranthene	17
1878	230	C_2-Pyrene/C_2-Fluoranthene	4

continued...

Table 6.5.5. Continued.

Scan	M/W	Compound	ppb
1915	228	Benzo(a)anthracene	3
1926	228	Chrysene/Triphenylene	61
1930	244	C_3-Pyrene/C_3-Fluoranthene	4
1938	244	C_3-Pyrene/C_3-Fluoranthene	4
1949	244	C_3-Pyrene/C_3-Fluoranthene	5
1960	244	C_3-Pyrene/C_3-Fluoranthene	6
1969	244	C_3-Pyrene/C_3-Fluoranthene	25
1992	244	C_3-Pyrene/C_3-Fluoranthene	6
2005	244	C_3-Pyrene/C_3-Fluoranthene	12
2017	244	C_3-Pyrene/C_3-Fluoranthene	6
2020	254	C_5-Dibenzothiophene	5
2024	244	C_3-Pyrene/C_3-Fluoranthene	10
2043	244	C_3-Pyrene/C_3-Fluoranthene	9
2045	268	C_6-Dibenzothiophene	2
2051	244	C_3-Pyrene/C_3-Fluoranthene	3
2060	244	C_3-Pyrene/C_3-Fluoranthene	3
2062	268	C_6-Dibenzothiophene	2
2066	244	C_3-Pyrene/C_3-Fluoranthene	2
2074	242	C_1-Chrysene/C_1-Triphenylene	36
2086	242	C_1-Chrysene/C_1-Triphenylene	15
2101	242	C_1-Chrysene/C_1-Triphenylene	10
2104	258	C_4-Pyrene/C_4-Fluoranthene	5
2111	258	C_4-Pyrene/C_4-Fluoranthene	3
2113	268	C_6-Dibenzothiophene	2
2118	242	C_1-Chrysene/C_1-Triphenylene	12
2131	268	C_6-Dibenzothiophene	2
2136	258	C_4-Pyrene/C_4-Fluoranthene	2
2145	258	C_4-Pyrene/C_4-Fluoranthene	7
2149	268	C_6-Dibenzothiophene	6
2166	268	C_6-Dibenzothiophene	2
2172	258	C_4-Pyrene/C_4-Fluoranthene	3
2181	258	C_4-Pyrene/C_4-Fluoranthene	3
2215	256	C_2-Chrysene/C_2-Triphenylene	13
2239	256	C_2-Chrysene/C_2-Triphenylene	14
2252	256	C_2-Chrysene/C_2-Triphenylene	5
2268	256	C_2-Chrysene/C_2-Triphenylene	9
2281	256	C_2-Chrysene/C_2-Triphenylene	4
2286	252	Benzofluoranthene	6
2320	256	C_2-Chrysene/C_2-Triphenylene	4
2333	258	C_4-Pyrene/C_4-Fluoranthene	13
2347	270	C_3-Chrysene/C_3-Triphenylene	2
2352	258	C_4-Pyrene/C_4-Fluoranthene	2
2354	270	C_3-Chrysene/C_3-Triphenylene	2
2365	252	Benzo(e)pyrene	14
2380	252	Benzo(a)pyrene	3
2386	270	C_3-Chrysene/C_3-Triphenylene	5

continued...

Table 6.5.5. Concluded.

Scan	M/W	Compound	ppb
2395	270	C_3-Chrysene/C_3-Triphenylene	7
2416	270	C_3-Chrysene/C_3-Triphenylene	5
2434	266	C_1-Benzofluoranthene/C_1-Benzopyrene/C_1-Perylene	2
2457	270	C_3-Chrysene/C_3-Triphenylene	3
2465	270	C_3-Chrysene/C_3-Triphenylene	4
2495	270	C_3-Chrysene/C_3-Triphenylene	8
2503	266	C_1-Benzofluoranthene/C_1-Benzopyrene/C_1-Perylene	4
2538	266	C_1-Benzofluoranthene/C_1-Benzopyrene/C_1-Perylene	6
2547	266	C_1-Benzofluoranthene/C_1-Benzopyrene/C_1-Perylene	3
2616	284	C_4-Chrysene/C_4-Triphenylene	2
2622	280	C_2-Benzofluoranthene/C_2-Benzopyrene/C_2-Perylene	3
2651	284	C_4-Chrysene/C_4-Triphenylene	4
2670	280	C_2-Benzofluoranthene/C_2-Benzopyrene/C_2-Perylene	4
2680	280	C_2-Benzofluoranthene/C_2-Benzopyrene/C_2-Perylene	1
2773	276	Benzo(ghi)perylene	3

APPENDIX 6.6

Aromatic and nitrogen components of UMATAC-produced oil.

Table 6.6.1. UMATAC overhead oil aromatic components, 1982 October.

Scan	M.W.	Compound	ppm
319	128	Naphthalene	581
325	134	Benzothiophene	287
425	148	C_1-Benzothiophene	137
437	142	C_1-Naphthalene	835
437	148	C_1-Benzothiophene	293
444	148	C_1-Benzothiophene	156
456	148	C_1-Benzothiophene	421
458	142	C_1-Naphthalene	681
554	162	C_2-Benzothiophene	224
563	156	C_2-Naphthalene	176
564	162	C_2-Benzothiophene	116
582	156	C_2-Naphthalene	417
583	162	C_2-Benzothiophene	345
593	162	C_2-Benzothiophene	474
604	156	C_2-Naphthalene	711
606	162	C_2-Benzothiophene	162
608	156	C_2-Naphthalene	278
613	162	C_2-Benzothiophene	202
615	154	Biphenyl	56
629	156	C_2-Naphthalene	332
633	156	C_2-Naphthalene	82
641	152	Acenaphthylene	101
651	156	C_2-Naphthalene	227
692	154	Acenaphthene	126
698	176	C_3-Benzothiophene	81
700	170	C_3-Naphthalene	23
714	170	C_3-Naphthalene	56
714	176	C_3-Benzothiophene	149
727	170	C_3-Naphthalene	99
729	176	C_3-Benzothiophene	262
735	176	C_3-Benzothiophene	198
736	170	C_3-Naphthalene	238
743	170	C_3-Naphthalene	32
752	176	C_3-Benzothiophene	287
754	170	C_3-Naphthalene	89
759	170	C_3-Naphthalene	173
764	176	C_3-Benzothiophene	34
766	170	C_3-Naphthalene	206
780	170	C_3-Naphthalene	64
780	176	C_3-Benzothiophene	49
788	176	C_3-Benzothiophene	22
791	170	C_3-Naphthalene	241
794	176	C_3-Benzothiophene	49
795	170	C_3-Naphthalene	142
805	176	C_3-Benzothiophene	47
817	190	C_4-Benzothiophene	42

continued...

Table 6.6.1. Continued.

Scan	M.W.	Compound	ppm
820	170	C_3-Naphthalene	272
833	176	C_3-Benzothiophene	38
840	170	C_3-Naphthalene	48
843	190	C_4-Benzothiophene	44
845	166	Fluorene	119
852	176	C_3-Benzothiophene	71
854	170	C_3-Naphthalene	172
854	190	C_4-Benzothiophene	97
861	190	C_4-Benzothiophene	36
865	168	C_1-Acenaphthene/C_1-Biphenyl	64
874	190	C_4-Benzothiophene	144
875	168	C_1-Acenaphthene/C_1-Biphenyl	118
881	180	C_1-Fluorene	29
883	170	C_3-Naphthalene	57
886	168	C_1-Acenaphthene/C_1-Biphenyl	60
888	190	C_4-Benzothiophene	39
897	190	C_4-Benzothiophene	37
907	190	C_4-Benzothiophene	43
916	190	C_4-Benzothiophene	55
941	190	C_4-Benzothiophene	52
956	190	C_4-Benzothiophene	28
973	190	C_4-Benzothiophene	40
984	204	C_5-Benzothiophene	17
992	204	C_5-Benzothiophene	17
994	190	C_4-Benzothiophene	14
996	180	C_1-Fluorene	7
1001	190	C_4-Benzothiophene	30
1013	190	C_4-Benzothiophene	36
1016	180	C_1-Fluorene	15
1028	180	C_1-Fluorene	73
1039	180	C_1-Fluorene	45
1049	204	C_5-Benzothiophene	17
1056	180	C_1-Fluorene	60
1065	204	C_5-Benzothiophene	14
1090	180	C_1-Fluorene	37
1094	204	C_5-Benzothiophene	12
1105	204	C_5-Benzothiophene	11
1108	184	Dibenzothiophene	104
1150	178	Phenanthrene	125
1151	204	C_5-Benzothiophene	12
1164	178	Anthracene	50
1188	194	C_2-Fluorene	15
1206	194	C_2-Fluorene	27
1215	194	C_2-Fluorene	20
1221	194	C_2-Fluorene	15
1229	194	C_2-Fluorene	17

continued...

Table 6.6.1. Continued.

Scan	M.W.	Compound	ppm
1250	194	C_2-Fluorene	27
1263	198	C_1-Dibenzothiophene	74
1264	194	C_2-Fluorene	11
1273	194	C_2-Fluorene	26
1276	198	C_1-Dibenzothiophene	14
1295	198	C_1-Dibenzothiophene	58
1306	198	C_1-Dibenzothiophene	21
1318	198	C_1-Dibenzothiophene	21
1326	192	C_1-Phenanthrene/C_1-Anthracene	28
1328	198	C_1-Dibenzothiophene	53
1346	192	C_1-Phenanthrene/C_1-Anthracene	28
1363	208	C_3-Fluorene	10
1369	192	C_1-Phenanthrene/C_1-Anthracene	38
1384	208	C_3-Fluorene	11
1393	208	C_3-Fluorene	8
1400	208	C_3-Fluorene	12
1412	212	C_2-Dibenzothiophene	24
1420	208	C_3-Fluorene	13
1432	208	C_3-Fluorene	13
1433	212	C_2-Dibenzothiophene	21
1440	212	C_2-Dibenzothiophene	16
1445	212	C_2-Dibenzothiophene	18
1446	208	C_3-Fluorene	8
1457	208	C_3-Fluorene	9
1463	206	C_2-Phenanthrene/C_2-Anthracene	7
1466	212	C_2-Dibenzothiophene	12
1479	208	C_3-Fluorene	11
1480	212	C_2-Dibenzothiophene	61
1488	206	C_2-Phenanthrene/C_2-Anthracene	14
1499	212	C_2-Dibenzothiophene	19
1502	206	C_2-Phenanthrene/C_2-Anthracene	12
1518	206	C_2-Phenanthrene/C_2-Anthracene	12
1529	206	C_2-Phenanthrene/C_2-Anthracene	39
1530	212	C_2-Dibenzothiophene	11
1537	206	C_2-Phenanthrene/C_2-Anthracene	25
1545	206	C_2-Phenanthrene/C_2-Anthracene	13
1554	206	C_2-Phenanthrene/C_2-Anthracene	7
1560	206	C_2-Phenanthrene/C_2-Anthracene	7
1561	202	Fluoranthene	8
1578	206	C_2-Phenanthrene/C_2-Anthracene	7
1578	226	C_3-Dibenzothiophene	18
1600	206	C_2-Phenanthrene/C_2-Anthracene	6
1608	226	C_3-Dibenzothiophene	13
1624	226	C_3-Dibenzothiophene	13
1631	202	Pyrene	12
1656	220	C_3-Phenanthrene/C_3-Anthracene	12

continued...

Table 6.6.1. Continued.

Scan	M.W.	Compound	ppm
1671	226	C_3-Dibenzothiophene	12
1683	220	C_3-Phenanthrene/C_3-Anthracene	9
1697	220	C_3-Phenanthrene/C_3-Anthracene	13
1707	226	C_3-Dibenzothiophene	10
1719	220	C_3-Phenanthrene/C_3-Anthracene	10
1757	220	C_3-Phenanthrene/C_3-Anthracene	5
1770	216	Benzo(a)fluorene	5
1798	216	Benzo(b)fluorene	5
1802	220	C_3-Penanthrene/C_3-Anthracene	8
1830	216	C_1-Pyrene	5
1837	216	C_1-Pyrene	3.5
1938	230	C_2-Pyrene, C_2-Fluoranthene/ C_1-Benzofluorene	4.3
1958	230	C_2-Pyrene, C_2-Fluoranthene/ C_1-Benzofluorene	3.6
1967	230	C_2-Pyrene, C_2-Fluoranthene/ C_1-Benzofluorene	1.3
1982	230	C_2-Pyrene, C_2-Fluoranthene/ C_1-Benzofluorene	1.8
1986	234	Benzonaphthothiophene	6.9
1991	230	C_2-Pyrene, C_2-Fluoranthene/ C_1-Benzofluorene	1.7
2000	230	C_2-Pyrene, C_2-Fluoranthene/ C_1-Benzofluorene	2.1
2010	230	Benzonaphthothiophene	3.3
2076	228	Benzo(a)anthracene	4.2
2087	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	1.2
2089	228	Chrysene/Triphenylene	9.6
2106	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	2.1
2120	248	C_1-Benzonaphthothiophene	4.6
2129	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3.1
2148	248	C_1-Benzonaphthothiophene	6.8
2166	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	1.7
2178	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	2.4
2184	248	C_1-Benzonaphthothiophene	10.6
2205	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	3.2
2209	248	C_1-Benzonaphthothiophene	6.2
2221	242	C_1-Benzo(a)anthracene/C_1-Chrysene/ C_1-Triphenylene	1.9

continued...

Table 6.6.1. Continued.

Scan	M.W.	Compound	ppm
2234	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	3.9
2246	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	4.7
2262	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	2.7
2268	262	C_2-Benzohaphthothiophene	6.2
2278	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	5.0
2398	256	C_2-Benzo(a)anthracene/C_2-Triphenylene/C_2-Chrysene	3.9
2300	262	C_2-Benzonaphthothiophene	3.0
2309	262	C_2-Benzonaphthothiophene	2.3
2315	262	C_2-Benzonaphthothiophene	2.3
2334	262	C_2-Benzonaphthothiophene	7.0
2359	262	C_2-Benzonaphthothiophene	3.7
2412	256	C_2-Benzo(a)anthracene/C_2-Triphenylene/C_2-Chrysene	1.8
2423	256	C_2-Benzo(a)anthracene/C_2-Triphenylene/C_2-Chrysene	1.5
2429	256	C_2-Benzo(a)anthracene/C_2-Triphenylene/C_2-Chrysene	2.1
2448	252	Benzofluoranthenes	3.2
2461	256	C_2-Benzo(a)anthracene/C_2-Triphenylene/C_2-Chrysene	1.8
2482	256	C_2-Benzo(a)anthracene/C_2-Triphenylene/C_2-Chrysene	1.5
2513	270	C_3-Benzo(a)anthracene/C_3-Chrysene/C_3-Triphenylene	1.8
2529	252	Benzo(e)pyrene	3.2
2537	270	C_3-Benzo(a)anthracene/C_3-Triphenylene/C_3-Chrysene	1.3
2543	252	Benzo(a)pyrene	2.9
2544	270	C_3-Benzo(a)anthracene/C_3-Triphenylene/C_3-Chrysene	1.3
2555	270	C_3-Benzo(a)anthracene/C_3-Triphenylene/C_3-Chrysene	2.0
2571	252	Perylene	1.2
2594	266	C_1-Benzo(a)pyrene/C_1-Benzofluranthenes/C_1-Benzo(e)pyrene/C_1-Perylene	1.3
2618	270	C_3-Benzo(a)anthracene/C_3-Triphenylene/C_3-Chrysene	2.0
2633	266	C_1-Benzo(a)pyrene/C_1-Benzoflurathenes/C_1-Benzo(e)pyrene/C_1-Perylene	1.8
2657	270	C_3-Benzo(a)anthracene/C_3-Triphenylene/C_3-Chrysene	1.4

continued...

Table 6.6.1. Concluded.

Scan	M.W.	Compound	ppm
2658	266	C_1-Benzo(a)pyrene/C_1-Benzo(e)pyrene/ C_1-Benzofluoranthenes/C_1-Perylene	1.0
2665	266	C_1-Benzo(a)pyrene/C_1-Benzo(e)pyrene/ C_1-Benzofluoranthenes/C_1-Perylene	1.1
2701	266	C_1-Benzo(a)pyrene/C_1-Benzo(e)pyrene/ C_1-Benzofluoranthenes/C_1-Perylene	1.6
2710	266	C_1-Benzo(a)pyrene/C_1-Benzo(e)pyrene/ C_1-Benzofluoranthenes/C_1-Perylene	1.1
2772	280	C_2-Benzo(a)pyrene/C_2-Benzo(e)pyrene/ C_2-Benzofluoranthenes/C_2-Perylene	1.0
2780	280	C_2-Benzo(a)pyrene/C_2-Benzo(e)pyrene/ C_2-Benzofluoranthenes/C_2-Perylene	1.7
2831	280	C_2-Benzo(a)pyrene/C_2-Benzo(e)pyrene/ C_2-Benzofluoranthenes/C_2-Perylene	1.3
2841	280	C_2-Benzo(a)pyrene/C_2-Benzo(e)pyrene/ C_2-Benzofluoranthenes/C_2-Perylene	0.6
2934	276	Benzo(ghi)perylene	1.1

Table 6.6.2. UMATAC overhead oil aromatic components, 1982 October.

Scan	M.W.	Compound	ppm
308	134	Benzo(b)thiophene	5.8
369	144	C_1-Dihydronaphthalene	68
374	144	C_1-Dihydronaphthalene	80
401	144	C_1-Dihydronaphthalene	23
407	142	2-Methylnaphthalene	260
408	148	C_1-Benzo(b)thiophene	100
417	148	C_1-Benzo(b)thiophene	45
425	148	C_1-Benzo(b)thiophene	150
426	142	1-Methylnaphthalene	210
471	158	C_2-Dihydronaphthalene	22
489	158	C_2-Dihydronaphthalene	18
494	158	C_2-Dihydronaphthalene	27
504	158	C_2-Dihydronaphthalene	47
511	154	1,1'-Biphenyl	56
522	162	C_2-Benzo(b)thiophene	120
530	156	C_2-Naphthalene	59
531	162	C_2-Benzo(b)thiophene	63
534	158	C_2-Dihydronaphthalene	39
535	162	C_2-Benzo(b)thiophene	26
535	156	C_2-Naphthalene	28
537	158	C_2-Dihydronaphthalene	50
545	156	C_2-Naphthalene	180
546	162	C_2-Benzo(b)thiophene	210
556	162	C_2-Benzo(b)thiophene	300
564	162	C_2-Benzo(b)thiophene	46
565	156	C_2-Naphthalene	230
567	162	C_2-Benzo(b)thiophene	77
570	156	C_2-Naphthalene	170
577	162	C_2-Benzo(b)thiophene	140
592	156	C_2-Naphthalene	120
597	156	C_2-Naphthalene	45
614	156	C_2-Naphthalene	81
631	162	C_2-Benzo(b)thiophene	21
662	168	C_1-Biphenyl	0.13
664	176	C_3-Benzo(b)thiophene	66
677	176	C_3-Benzo(b)thiophene	130
689	170	C_3-Naphthalene	59
690	176	C_3-Benzo(b)thiophene	180
696	176	C_3-Benzo(b)thiophene	200
714	176	C_3-Benzo(b)thiophene	220
721	170	C_3-Naphthalene	70
727	176	C_3-Benzo(b)thiophene	29
728	170	C_3-Naphthalene	100
740	176	C_3-Benzo(b)thiophene	170
746	168	C_1-Biphenyl	18
753	170	C_3-Naphthalene	110
757	170	C_3-Naphthalene	77
769	176	C_3-Benzo(b)thiophene	41

continued...

Table 6.6.2. Continued.

Scan	M.W.	Compound	ppm
780	190	C_4-Benzo(b)thiophene	21
782	170	C_3-Naphthalene	170
797	176	C_3-Benzo(b)thiophene	32
804	170	C_3-Naphthalene	28
806	166	Fluorene	110
813	176	C_3-Benzo(b)thiophene	67
816	170	C_3-Naphthalene	80
816	190	C_4-Benzo(b)thiophene	80
825	190	C_4-Benzo(b)thiophene	34
829	168	C_1-Biphenyl	63
835	168	C_1-Biphenyl	110
837	190	C_4-Benzo(b)thiophene	90
841	190	C_4-Benzo(b)thiophene	47
843	170	C_3-Naphthalene	31
847	168	C_1-Biphenyl	49
852	190	C_4-Benzo(b)thiophene	35
862	190	C_4-Benzo(b)thiophene	35
869	182	C_2-Biphenyl	39
871	190	C_4-Benzo(b)thiophene	47
878	184	C_4-Naphthalene	18
881	190	C_4-Benzo(b)thiophene	54
905	190	C_4-Benzo(b)thiophene	40
908	190	C_4-Benzo(b)thiophene	23
914	184	C_4-Naphthalene	45
921	190	C_4-Benzo(b)thiophene	31
937	190	C_4-Benzo(b)thiophene	60
947	184	C_4-Naphthalene	43
949	204	C_5-Benzo(b)thiophene	23
958	204	C_5-Benzo(b)thiophene	21
964	190	C_4-Benzo(b)thiophene	49
972	184	C_4-Naphthalene	47
976	204	C_5-Benzo(b)thiophene	40
979	184	C_4-Naphthalene	26
984	190	C_5-Benzo(b)thiophene	68
986	180	C_1-Fluorene	38
989	180	1-Methylfluorene	51
999	180	2-Methylfluorene	64
1004	184	C_4-Naphthalene	21
1017	194	C_2-Fluorene	28
1019	184	C_4-Naphthalene	27
1026	182	C_2-Biphenyl	25
1031	182	C_2-Biphenyl	30
1041	182	C_2-Biphenyl	42
1045	184	C_4-Naphthalene	30
1051	182	C_2-Biphenyl	22
1068	184	Dibenzothiophene	120
1075	182	C_2-Biphenyl	38
1110	178	Phenanthrene	130

continued...

Table 6.6.2. Continued.

Scan	M.W.	Compound	ppm
1114	204	C_5-Benzo(b)thiophene	15
1125	178	Anthracene	52
1169	194	C_2-Fluorene	41
1177	194	C_2-Fluorene	34
1182	194	C_2-Fluorene	20
1189	194	C_2-Fluorene	38
1197	194	C_2-Fluorene	12
1204	208	C_3-Fluorene	11
1211	194	C_2-Fluorene	51
1224	198	C_1-Dibenzothiophene	100
1235	194	C_2-Fluorene	25
1238	198	C_1-Dibenzothiophene	22
1255	198	C_1-Dibenzothiophene	77
1267	198	C_1-Dibenzothiophene	40
1280	198	C_1-Dibenzothiophene	19
1287	192	C_1-Phenanthrene/C_1-Anthracene	43
1289	198	C_1-Dibenzothiophene	78
1295	192	C_1-Phenathrene/C_1-Anthracene	73
1309	192	C_1-Phenathrene/C_1-Anthracene	29
1324	192	C_1-Phenathrene/C_1-Anthracene	80
1327	208	C_3-Fluorene	19
1331	192	1-Methylphenanthrene	52
1348	208	C_3-Fluorene	23
1358	208	C_3-Fluorene	14
1365	208	C_3-Fluorene	22
1365	212	C_2-Dibenzothiophene	11
1376	212	C_2-Dibenzothiophene	34
1388	222	C_4-Fluorene	3.6
1395	208	C_3-Fluorene	17
1397	212	C_2-Dibenzothiophene	24
1405	212	C_2-Dibenzothiophene	24
1409	212	C_2-Dibenzothiophene	25
1416	212	C_2-Dibenzothiophene	11
1422	208	C_3-Fluorene	10
1431	212	C_2-Dibenzothiophene	17
1443	212	C_2-Dibenzothiophene	91
1443	208	C_3-Fluorene	18
1453	206	C_2-Phenanthrene/C_2-Anthracene	14
1464	212	C_2-Dibenzothiophene	35
1467	206	C_2-Phenanthrene/C_2-Anthracene	13
1471	212	C_2-Dibenzothiophene	13
1473	206	C_2-Phenanthrene/C_2-Anthracene	8.2
1484	206	C_2-Phenanthrene/C_2-Anthracene	16
1493	206	C_2-Phenanthrene/C_2-Anthracene	56
1502	206	C_2-Phenanthrene/C_2-Anthracene	35
1510	206	C_2-Phenanthrene/C_2-Anthracene	22
1520	206	C_2-Phenanthrene/C_2-Anthracene	8.5
1525	202	Fluoranthene	7.8

continued...

Table 6.6.2. Concluded.

Scan	M.W.	Compound	ppm
1526	206	C_2-Phenanthrene/C_2-Anthracene	9.7
1597	202	Pyrene	15
1625	220	C_3-Phenanthrene/C_3-Anthracene	3.3
1652	220	C_3-Phenanthrene/C_3-Anthracene	11
1664	220	C_3-Phenanthrene/C_3-Anthracene	17
1687	220	C_3-Phenanthrene/C_3-Anthracene	7.2
1798	216	C_1-Pyrene/C_1-Fluoranthene	2.5
1807	216	C_1-Pyrene/C_1-Fluoranthene	1.4

Table 6.6.3. UMATAC sidedraw oil aromatic components, 1982 October.

Scan	M.W.	Compound	ppm
328	142	C_1-Dihydronaphthalene	83
350	148	C_1-Benzo(b)thiophene	26
357	142	2-Methylnaphthalene	290
358	148	C_1-Benzo(b)thiophene	57
366	148	C_1-Benzo(b)thiophene	28
373	148	C_1-Benzo(b)thiophene	83
374	142	1-Methylnaphthalene	235
416	158	C_2-Dihydronaphthalene	22
453	154	Biphenyl	19
462	162	C_2-Benzo(b)thiophene	59
470	156	C_2-Naphthalene	69
471	162	C_2-Benzo(b)thiophene	44
477	158	C_2-Dihydronaphthalene	38
484	156	C_2-Naphthalene	120
485	162	C_2-Benzo(b)thiophene	110
495	162	C_2-Benzo(b)thiophene	140
503	156	C_2-Naphthalene	160
505	162	C_2-Benzo(b)thiophene	62
507	156	C_2-Naphthalene	130
513	162	C_2-Benzo(b)thiophene	67
516	154	Dihydroethenonaphthalene	22
528	156	C_2-Naphthalene	120
545	172	C_3-Dihydronaphthalene	11
549	156	C_2-Napthalene	60
590	154	Acenaphthene	67
609	176	C_3-Benzo(b)thiophene	74
620	170	C_3-Naphthalene	57
620	176	C_3-Benzo(b)thiophene	110
626	176	C_3-Benzo(b)thiophene	130
642	176	C_3-Benzo(b)thiophene	150
652	170	C_3-Naphthalene	58
657	170	C_3-Naphthalene	100
668	176	C_3-Benzo(b)thiophene	110
680	170	C_3-Naphthalene	150
708	170	C_3-Naphthalene	140
732	166	Fluorene	94
740	176	C_3-Benzo(b)thiophene	57
741	170	C_3-Naphthalene	79
742	190	C_4-Benzo(b)thiophene	87
754	168	Propenylnaphthalene	69
760	168	Propenylnaphthalene	100
762	190	C_4-Benzo(b)thiophene	190
771	168	Propenylnaphthalene	60
786	190	C_4-Benzo(b)thiophene	41
794	190	C_4-Benzo(b)thiophene	45
803	190	C_4-Benzo(b)thiophene	75
858	190	C_4-Benzo(b)thiophene	50
868	184	C_4-Naphthalene	57

continued...

Table 6.6.3. Continued.

Scan	M.W.	Compound	ppm
878	204	C_5-Benzo(b)thiophene	51
884	190	C_4-Benzo(b)thiophene	54
892	184	C_4-Naphthalene	65
898	204	C_5-Benzo(b)thiophene	100
904	190	C_4-Benzo(b)thiophene	79
908	180	C_1-Fluorene	94
917	180	C_1-Fluorene	78
933	180	C_1-Fluorene	84
934	182	C_2-Biphenyl/C_2-Acenaphthene	63
949	182	C_2-Biphenyl/C_2-Acenaphthene	34
959	182	C_2-Biphenyl/C_2-Acenaphthene	50
962	184	C_4-Naphthalene	53
967	182	C_2-Biphenyl/C_2-Acenaphthene	10
973	196	C_3-Biphenyl/C_3-Acenaphthene	59
984	184	Dibenzothiophene	150
991	182	C_2-Biphenyl/C_2-Acenaphthene	50
1007	196	C_3-Biphenyl/C_3-Acenaphthene	64
1020	196	C_3-Biphenyl/C_3-Acenaphthene	39
1026	178	Phenanthrene	200
1032	204	C_5-Benzo(b)thiophene	55
1037	196	C_3-Biphenyl/C_3-Acenaphthene	32
1041	178	Anthracene	71
1043	210	C_4-Biphenyl/C_4-Acenaphthene	41
1075	196	C_3-Biphenyl/C_3-Acenaphthene	33
1086	194	C_2-Fluorene	59
1094	194	C_2-Fluorene	87
1104	210	C_4-Biphenyl/C_4-Acenaphthene	54
1106	194	C_2-Fluorene	69
1127	194	C_2-Fluorene	81
1127	208	C_3-Fluorene	40
1135	196	C_3-Biphenyl/C_3-Acenaphthene	47
1139	198	C_1-Dibenzothiophene	180
1152	194	C_2-Fluorene	68
1162	196	C_3-Biphenyl/C_3-Acenaphthene	65
1170	196	C_3-Biphenyl/C_3-Acenaphthene	56
1170	198	C_1-Dibenzothiophene	130
1183	198	C_1-Dibenzothiophene	46
1196	198	C_1-Dibenzothiophene	44
1201	196	C_3-Biphenyl/C_3-Acenaphthene	51
1203	192	C_1-Phenanthrene/C_1-Anthracene	100
1204	198	C_1-Dibenzothiophene	160
1211	192	C_1-Phenanthrene/C_1-Anthracene	170
1219	210	C_4-Biphenyl/C_4-Acenaphthene	55
1224	192	C_1-Phenanthrene/C_1-Anthracene	78
1239	192	C_1-Phenanthrene/C_1-Anthracene	200
1243	208	C_3-Fluorene	72
1245	192	C_1-Phenanthrene/C_1-Anthracene	140
1264	208	C_3-Fluorene	75

continued...

Table 6.6.3. Continued.

Scan	M.W.	Compound	ppm
1280	212	C_2-Dibenzothiophene	49
1282	208	C_3-Fluorene	60
1291	212	C_2-Dibenzothiophene	130
1311	208	C_3-Fluorene	65
1313	212	C_2-Dibenzothiophene	98
1324	212	C_2-Dibenzothiophene	190
1337	208	C_3-Fluorene	50
1345	212	C_2-Dibenzothiophene	71
1347	210	C_4-Biphenyl/C_4-Acenaphthene	62
1356	212	C_2-Dibenzothiophene	390
1358	208	C_3-Fluorene	91
1367	206	C_2-Phenanthrene/C_2-Anthracene	75
1376	212	C_2-Dibenzothiophene	150
1382	206	C_2-Phenanthrene/C_2-Anthracene	64
1384	212	C_2-Dibenzothiophene	66
1387	206	C_2-Phenanthrene/C_2-Anthracene	35
1399	206	C_2-Phenanthrene/C_2-Anthracene	76
1407	206	C_2-Phenanthrene/C_2-Anthracene	270
1408	212	C_2-Dibenzothiophene	91
1416	206	C_2-Phenanthrene/C_2-Anthracene	190
1424	206	C_2-Phenanthrene/C_2-Anthracene	110
1424	226	C_3-Dibenzothiophene	77
1434	206	C_2-Phenanthrene/C_2-Anthracene	45
1438	202	Fluoranthene	91
1439	206	C_2-Phenanthrene/C_2-Anthracene	70
1439	212	C_2-Dibenzothiophene	94
1458	206	C_2-Phenanthrene/C_2-Anthracene	87
1459	226	C_3-Dibenzothiophene	220
1479	206	C_2-Phenanthrene/C_2-Anthracene	79
1488	226	C_3-Dibenzothiophene	230
1504	226	C_3-Dibenzothiophene	220
1508	202	Pyrene	180
1523	226	C_3-Dibenzothiophene	140
1530	226	C_3-Dibenzothiophene	170
1537	220	C_3-Phenanthrene/C_3-Anthracene	140
1545	226	C_3-Dibenzothiophene	110
1551	226	C_3-Dibenzothiophene	120
1566	220	C_3-Phenanthrene/C_3-Anthracene	190
1578	220	C_3-Phenanthrene/C_3-Anthracene	280
1587	226	C_3-Dibenzothiophene	150
1600	220	C_3-Phenanthrene/C_3-Anthracene	200
1606	226	C_3-Dibenzothiophene	81
1621	240	C_4-Dibenzothiophene	95
1628	240	C_4-Dibenzothiophene	80
1638	220	C_3-Phenanthrene/C_3-Anthracene	100
1648	220	C_3-Phenanthrene/C_3-Anthracene	91
1649	216	Benzo(a)fluorene	79
1677	216	Benzo(b)fluorene	110

continued...

Table 6.6.3. Continued.

Scan	M.W.	Compound	ppm
1682	220	C_3-Phenanthrene/C_3-Anthracene	200
1698	240	C_4-Dibenzothiophene	94
1708	216	C_1-Pyrene	130
1709	218	C_1-Dihydropyrene	230
1717	216	C_1-Pyrene	82
1721	240	C_4-Dibenzothiophene	140
1742	240	C_4-Dibenzothiophene	98
1748	234	C_4-Phenanthrene	94
1756	232	C_2-Dihydropyrene	100
1769	216	C_1-Pyrene	30
1769	232	C_2-Dihydropyrene	130
1813	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzfluorene	55
1818	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzfluorene	46
1838	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzfluorene	56
1860	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzfluorene	46
1864	234	Benzonaphthothiophene	130
1896	234	Benzonaphthothiophene	72
1908	230	C_2-Pyrene	66
1954	228	Benzo(a)anthracene	55
1964	246	C_3-Dihydropyrene	84
1966	228	Chrysene/Triphenylene	150
1976	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzfluorene	19
1997	248	C_1-Benzonaphthothiophene	120
2012	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzfluorene	130
2025	248	C_1-Benzonaphthothiophene	140
2032	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzfluorene	36
2060	248	C_1-Benzonaphthothiophene	220
2085	248	C_1-Benzonaphthothiophene	100
2095	242	C_1-Benzanthracene	10
2100	242	C_1-Benzanthracene	11
2112	242	C_1-Benzanthracene/C_1-Chrysene/ C_1-Triphenylene	130
2124	242	C_1-Benzanthracene/C_1-Chrysene/ C_1-Triphenylene	75
2140	242	C_1-Benzanthracene/C_1-Chrysene/ C_1-Triphenylene	35
2145	262	C_2-Benzonaphthothiophene	110
2146	242	C_1-Benzanthracene/C_1-Chrysene C_1-Triphenylene	16
2156	242	C_1-Benzanthracene/C_1-Chrysene/ C_1-Triphenylene	51

continued...

Table 6.6.3. Concluded.

Scan	M.W.	Compound	ppm
2180	242	C_1-Chrysene/C_1-Triphenylene	12
2190	262	C_2-Benzonaphthothiophene	190
2213	262	C_2-Benzonaphthothiophene	180
2251	256	C_2-Benzanthracene/C_2-Chrysene C_2-Triphenylene	59
2264	256	C_2-Benzanthracene/C_2-Chrysene/ C_2-Triphenylene	16
2275	256	C_2-Benzanthracene/C_2-Chrysene/ C_2-Triphenylene	54
2290	256	C_2-Benzanthracene/C_2-Chrysene/ C_2-Triphenylene	27
2298	256	C_2-Benzanthracene/C_2-Chrysene/ C_2-Triphenylene	25
2305	256	C_2-Benzanthracene/C_2-Chrysene/ C_2-Triphenylene	39
2315	276	C_3-Benzonaphthothiophene	99
2318	256	C_2-Chrysene/C_2-Triphenylene	14
2322	252	Benzo(b)fluoranthene	24
2336	256	C_2-Chrysene/C_2-Triphenylene	28
2340	276	C_3-Benzonaphthothiophene	130
2358	256	C_2-Chrysene/C_2-Triphenylene	26
2382	270	C_3-Benzanthracene/C_3-Chrysene/ C_3-Triphenylene	8.7
2389	270	C_3-Benzanthracene/C_3-Chrysene/ C_3-Triphenylene	17
2397	270	C_3-Benzanthracene/C_3-Chrysene/ C_3-Triphenylene	12
2400	252	Benzo(e)pyrene	44
2406	270	C_3-Benzanthracene/C_3-Chrysene/ C_3-Triphenylene	8.8
2409	266	C_1-Benzofluoranthene/ C_1-Benzo(e)pyrene	14
2412	270	C_3-Chrysene/C_3-Triphenylene	16
2415	252	Benzo(a)pyrene	32
2420	270	C_3-Chrysene/C_3-Triphenylene	25
2430	270	C_3-Chrysene/C_3-Triphenylene	38
2442	252	Perylene	18
2452	270	C_3-Chrysene/C_3-Triphenylene	18

Table 6.6.4. UMATAC sidedraw oil nitrogen components, 1982 October.

Scan	M.W.	Compound	ppm
457	135	C_3-Aniline	6.8
495	143	?	7.3
521	135	C_3-Aniline	28
531	157	C_1-Naphthylamine	1.9
552	157	C_1-Naphthylamine	2.0
583	157	C_2-Quinoline or C_1-Naphthylamine	26
594	157	C_2-Quinoline or C_1-Naphthylamine	2.3
601	157	C_2-Quinoline or C_1-Naphthylamine	2.0
620	143	C_1-Quinoline or Naphthylamine	2.4
647	145	C_2-Indole	5.5
653	157	C_2-Quinoline	10
655	145	C_2-Indole	3.9
681	171	C_3-Quinoline	8.3
698	144	C_1-Cinnoline	13
714	157	C_2-Quinoline	3.6
749	171	C_3-Quinoline	23
753	171	C_3-Quinoline	19
754	159	C_3-Indole	2.7
758	159	C_3-Indole	2.3
768	159	C_3-Indole	5.4
805	159	C_3-Indole	6.5
841	185	C_4-Quinoline	5.0
849	158	C_2-Cinnoline	5.4
856	171	C_3-Quinoline	11
881	173	C_4-Indole	2.9
891	185	C_4-Quinoline	7.1
908	185	C_4-Quinoline	2.8
919	173	C_4-Indole	3.7
957	185	C_4-Quinoline	4.2
962	185	C_4-Quinoline	4.3
973	173	C_4-Indole	2.5
978	185	C_4-Quinoline	9.0
985	173	C_4-Indole	2.8
997	185	C_4-Quinoline	2.0
1030	185	C_4-Quinoline	4.8
1034	185	C_4-Quinoline	4.2
1056	169	4-Aminobiphenyl	17
1066	183	C_1-Aminobiphenyl	9.6
1086	181	Aminofluorene	4.7
1128	183	C_1-Aminobiphenyl	4.3
1135	183	C_1-Aminobiphenyl	8.1
1139	195	C_1-Aminofluorene	9.6
1160	179	Benzo(f)quinoline	3.1
1182	195	C_1-Aminofluorene	3.4
1185	167	Carbazole	13
1245	197	C_2-Aminobiphenyl	9.6
1274	180	Benzo(c)cinnoline	28
1301	181	C_1-Carbazole	23

continued...

Table 6.6.4. Continued.

Scan	M.W.	Compound	ppm
1310	197	C_2-Aminobiphenyl	13
1323	209	C_2-Aminofluorene	4.6
1340	193	C_1-Benzoquinoline	3.2
1348	181	C_1-Carbazole	7.6
1355	181	C_1-Carbazole	8.9
1373	209	C_2-Aminofluorene	6.3
1375	181	C_1-Carbazole	16
1380	181	2-Aminofluorene	6.6
1391	195	C_2-Carbazole	18
1426	207	C_1-Aminophenanthrene/ C_1-Aminoanthracene	12
1448	194	C_1-Benzo(c)cinnoline	6.8
1458	195	C_2-Carbazole	12
1458	194	C_1-Benzo(c)cinnoline	16
1462	209	C_2-Aminofluorene	5.7
1463	195	C_2-Carbazole	10
1469	195	C_2-Carbazole	12
1484	195	C_2-Carbazole	17
1488	195	C_2-Carbazole	14
1509	194	C_1-Benzo(c)cinnoline	5.1
1512	207	C_2-Benzoquinoline	5.2
1514	194	C_1-Benzo(c)cinnoline	3.5
1519	194	C_1-Benzo(c)cinnoline	5.3
1520	195	C_2-Carbazole	20
1528	194	C_1-Benzo(c)cinnoline	4.8
1549	209	C_3-Carbazole	21
1564	207	C_2-Benzoquinoline	3.3
1570	209	C_3-Carbazole	31
1585	221	C_3-Benzoquinoline	3.7
1601	221	C_3-Benzoquinoline	4.2
1615	221	C_3-Benzoquinoline	3.9
1619	221	C_3-Benzoquinoline	0.78
1623	208	C_2-Benzo(c)cinnoline	5.2
1634	221	C_3-Benzoquinoline	5.7
1644	209	C_3-Carbazole	23
1648	223	C_3-Aminofluorene	4.2
1664	223	C_4-Carbazole	12
1666	221	C_3-Benzoquinoline	2.7
1674	221	C_3-Benzoquinoline	2.4
1679	208	C_2-Benzo(c)cinnoline	2.7
1685	221	C_3-Benzoquinoline	2.3
1692	221	C_3-Benzoquinoline	1.5
1700	223	C_4-Carbazole	8.2
1710	223	C_4-Carbazole	23
1719	193	2-Aminoanthracene	2.1
1727	217	Aminopyrene/Aminofluoranthene	3.1
1742	223	C_4-Carbazole	15
1754	221	C_3-Benzoquinoline	2.0

continued...

Table 6.6.4. Concluded.

Scan	M.W.	Compound	ppm
1759	223	C_4-Carbazole	10
1774	223	C_4-Carbazole	26
1781	223	C_4-Carbazole	18
1818	223	C_4-Carbazole	6.3
1824	237	C_5-Carbazole	6.7
1830	223	C_4-Carbazole	7.3
1864	237	C_5-Carbazole	12
1906	237	C_5-Carbazole	15
1976	237	C_5-Carbazole	9.8
2110	231	C_1-Benzocarbazole	3.8
2114	217	3-Aminofluoranthene	1.7
2161	217	1-Aminopyrene	51
2247	245	C_2-Benzocarbazole	4.5
2272	245	C_2-Benzocarbazole	8.3
2294	245	C_2-Benzocarbazole	4.4
2349	245	C_2-Benzocarbazole	7.5
2877	267	Dibenzocarbazole	1.3

Table 6.6.5.1. UMATAC overhead oil nitrogen components, 1982 October.

Scan	M.W.	Compound	ppm
364	117	Indole	1.2
448	131	C_1-Indole	0.41
474	131	C_1-Indole	0.43
482	131	C_1-Indole	0.48
573	131	C_1-Indole	0.28
576	145	C_2-Indole	0.70
610	145	C_2-Indole	0.66
640	145	C_2-Indole	0.33
1142	167	Carbazole	2.9
1257	181	C_1-Carbazole	4.1
1303	181	C_1-Carbazole	0.92
1311	181	C_1-Carbazole	0.90
1327	181	C_1-Carbazole	1.3
1346	195	C_2-Carbazole	2.6
1367	195	C_2-Carbazole	0.46
1412	195	C_2-Carbazole	1.1
1417	195	C_2-Carbazole	0.91
1423	195	C_2-Carbazole	1.0
1437	195	C_2-Carbazole	1.4
1442	195	C_2-Carbazole	1.1
1445	209	C_3-Carbazole	1.0
1474	195	C_2-Carbazole	0.61
1502	209	C_3-Carbazole	1.6
1524	209	C_3-Carbazole	1.9
1541	209	C_3-Carbazole	0.26
1547	209	C_3-Carbazole	0.32
1561	209	C_3-Carbazole	0.60
1567	209	C_3-Carbazole	0.35
1572	209	C_3-Carbazole	0.28
1580	209	C_3-Carbazole	0.65
1597	209	C_3-Carbazole	0.76
1617	223	C_4-Carbazole	0.43
1622	223	C_4-Carbazole	0.15
1634	223	C_4-Carbazole	0.22
1652	223	C_4-Carbazole	0.42
1663	223	C_4-Carbazole	0.93
1694	223	C_4-Carbazole	0.29
1709	237	C_5-Carbazole	0.16
1711	223	C_4-Carbazole	0.25
1727	223	C_4-Carbazole	0.57
1733	223	C_4-Carbazole	0.35
1737	237	C_5-Carbazole	0.086
1745	237	C_5-Carbazole	0.14
1752	237	C_5-Carbazole	0.092
1775	237	C_5-Carbazole	0.20
1845	251	C_6-Carbazole	0.044
1847	251	C_6-Carbazole	0.034
1858	237	C_5-Carbazole	0.29
1895	251	C_6-Carbazole	0.028

continued...

Table 6.6.5.1. Concluded.

Scan	M.W.	Compound	ppm
1905	251	C_6-Carbazole	0.029
1927	237	C_5-Carbazole	0.091
1934	251	C_6-Carbazole	0.021
1964	251	C_6-Carbazole	0.028
2173	231	C_1-Benzocarbazole	0.036
2244	245	C_2-Benzocarbazole	0.048
2357	259	C_3-Benzocarbazole	0.067
2364	259	C_3-Benzocarbazole	0.069
2434	259	C_3-Benzocarbazole	0.046

Table 6.6.5.2. UMATAC overhead oil nitrogen components, 1982 October.

Scan	M.W.	Compound	ppm
592	157	C_1-Naphthylamine/C_2-Quinoline	0.050
617	157	C_1-Naphthylamine/C_2-Quinoline	0.087
670	157	C_1-Naphthylamine/C_2-Quinoline	0.16
698	171	C_2-Naphthylamine/C_3-Quinoline	0.41
711	171	C_2-Naphthylamine/C_3-Quinoline	0.083
733	158	C_2-Cinnoline	0.28
756	171	C_2-Naphthylamine/C_3-Quinoline	0.094
766	171	C_2-Naphthylamine/C_3-Quinoline	0.16
781	171	C_2-Naphthylamine/C_3-Quinoline	0.23
786	171	C_2-Naphthylamine/C_3-Quinoline	0.057
798	171	C_2-Naphthylamine/C_3-Quinoline	0.078
809	171	C_2-Naphthylamine/C_3-Quinoline	0.14
828	169	2-Aminobiphenyl	0.71
853	171	C_2-Naphthylamine/C_3-Quinoline	0.095
861	185	C_2-Naphthylamine/C_3-Quinoline	0.78
875	171	C_2-Naphthylamine/C_3-Quinoline	0.13
877	184	1,1-Diphenylhydrazine	0.38
880	185	C_3-Naphthylamine	0.27
886	183	C_1-Aminobiphenyl	0.14
897	184	Diaminobiphenyl	0.30
912	185	C_4-Quinoline	1.0
915	185	C_3-Quinoline	0.60
927	185	C_4-Quinoline	0.14
938	172	C_3-Cinnoline	0.24
942	185	C_4-Quinoline	0.14
978	185	C_4-Quinoline	0.71
982	185	C_4-Quinoline	0.12
985	199	C_4-Naphthylamine/C_5-Quinoline	0.14
999	199	C_5-Quinoline	0.58
1030	172	C_3-Cinnoline	0.23
1032	183	C_1-Aminobiphenyl	0.15
1034	199	C_4-Naphthylamine/C_5-Quinoline	0.32
1041	198	C_1-Diaminobiphenyl	0.29
1046	199	C_4-Naphthylamine/C_5-Quinoline	0.15
1057	197	C_2-Aminobiphenyl	0.17
1066	199	C_4-Naphthylamine/C_5-Quinoline	0.55
1078	198	C_1-Diaminobiphenyl	0.22
1079	169	4-Aminobiphenyl	8.9
1109	183	C_1-Aminobiphenyl	0.095
1120	199	C_4-Naphthylamine/C_5-Quinoline	0.14
1128	179	Benzoquinoline	0.14
1137	185	C_4-Quinoline	0.27
1142	199	C_4-Naphthylamine	0.70
1149	179	Acridine	0.033
1158	183	C_1-Aminobiphenyl	0.20
1173	198	C_2-Aminobiphenyl	0.38
1181	179	Phenanthridine/Benzo(f)quinoline	0.61
1193	197	C_2-Aminobiphenyl	0.15

continued...

Table 6.6.5.2. Concluded.

Scan	M.W.	Compound	ppm
1198	199	C_5-Quinoline	0.17
1236	194	Unknown	0.14
1240	211	C_3-Aminobiphenyl	0.23
1268	197	C_2-Aminobiphenyl	0.36
1289	211	C_3-Aminobiphenyl	0.15
1298	180	Benzo(c)cinnoline	2.1
1315	193	C_1-Benzoquinoline	0.12
1316	211	C_3-Aminobiphenyl	0.14
1342	194	C_1-Benzo(c)cinnoline	0.29
1345	211	C_3-Aminobiphenyl	0.24
1358	211	C_3-Aminobiphenyl	0.086
1363	193	C_1-Benzoquinoline	0.14
1395	194	C_1-Benzo(c)cinnoline	0.67
1406	181	2-Aminofluorene	0.24
1450	207	C_2-Benzoquinoline	0.093
1464	211	C_3-Aminobiphenyl	0.059
1471	194	C_1-Benzo(c)cinnoline	0.37
1482	194	C_1-Benzo(c)cinnoline	0.42
1566	208	C_2-Benzo(c)cinnoline	0.046
1568	208	C_2-Benzo(c)cinnoline	0.050
1573	208	C_2-Benzo(c)cinnoline	0.087
1575	208	C_2-Benzo(c)cinnoline	0.062
2140	217	3-Aminofluoranthene	0.16
2189	217	Aminopyrene/Aminofluoranthene	18.0

APPENDIX 6.7

Aromatic components of oils produced from combustion tube experiments.

Table 6.7.1. Combustion tube oil 159-11, aromatic components, 1983 November.

Scan	m.w.	Compound	ppm
424	142	2-Methylnaphthalene	43.3
425	148	C_1-Benzothiophene	14.8
434	148	C_1-Benzothiophene	8.8
443	148	C_1-Benzothiophene	39.9
444	142	1-Methylnaphthalene	36.0
542	162	C_2-Benzothiophene	26.2
549	156	C_2-Naphthalene	8.8
551	162	C_2-Benzothiophene	17.2
564	156	C_2-Naphthalene	36.1
566	162	C_2-Benzothiophene	49.2
576	162	C_2-Benzothiophene	64.5
586	156	C_2-Naphthalene	42.2
588	162	C_2-Benzothiophene	30.2
590	156	C_2-Naphthalene	48.6
597	162	C_2-Benzothiophene	24.2
613	156	C_2-Naphthalene	19.9
618	156	C_2-Naphthalene	11.5
636	156	C_2-Naphthalene	13.6
679	154	Acenaphthalene	8.3
684	176	C_3-Benzothiophene	14.1
699	176	C_3-Benzothiophene	23.2
711	170	C_3-Naphthalene	11.8
712	176	C_3-Benzothiophene	36.8
717	176	C_3-Benzothiophene	23.2
719	170	C_3-Naphthalene	11.0
725	176	C_3-Benzothiophene	8.0
736	176	C_3-Benzothiophene	46.1
743	170	C_3-Naphthalene	15.4
751	170	C_3-Naphthalene	25.1
763	176	C_3-Benzothiophene	32.3
775	170	C_3-Naphthalene	21.6
778	176	C_3-Benzothiophene	9.0
779	170	C_3-Naphthalene	16.0
802	176	C_3-Benzothiophene	7.9
804	170	C_3-Naphthalene	37.6
818	176	C_3-Benzothiophene	9.4
829	166	Fluorene	12.2
836	176	C_3-Benzothiophene	10.4
838	170	C_3-Naphthalene	27.8
851	168	C_1-Biphenyl	7.6
857	184	C_4-Naphthalene	8.0
858	168	C_1-Biphenyl	12.4
891	182	C_2-Biphenyl	7.8
910	182	C_2-Biphenyl	8.7
968	184	C_4-Naphthalene	9.5
994	184	C_4-Naphthalene	8.5

continued...

Table 6.7.1. Continued.

Scan	m.w.	Compound	ppm
1010	180	C_1-Fluorene	10.0
1020	180	C_1-Fluorene	9.7
1037	180	C_1-Fluorene	9.4
1066	184	C_4-Naphthalene	7.3
1090	184	Dibenzothiophene	35.1
1131	184	C_4-Naphthalene	10.4
1132	178	Phenanthrene	43.1
1147	178	Anthracene	12.2
1246	198	C_1-Dibenzothiophene	30.8
1279	198	C_1-Dibenzothiophene	21.9
1290	198	C_1-Dibenzothiophene	18.0
1311	192	C_1-Phenanthrene	19.4
1312	198	C_1-Dibenzothiophene	26.6
1319	192	C_1-Phenanthrene/C_1-Anthracene	34.2
1332	192	C_1-Phenanthrene/C_1-Anthracene	10.4
1348	192	C_1-Phenanthrene/C_1-Anthracene	39.2
1352	198	C_1-Dibenzothiophene	8.3
1355	192	C_1-Phenanthrene/C_1-Anthracene	18.1
1400	212	C_2-Dibenzothiophene	13.7
1422	212	C_2-Dibenzothiophene	9.4
1428	212	C_2-Dibenzothiophene	8.1
1433	212	C_2-Dibenzothiophene	17.9
1467	212	C_2-Dibenzothiophene	67.6
1477	206	C_2-Phenanthrene/C_2-Anthracene	15.1
1487	212	C_2-Dibenzothiophene	13.0
1492	206	C_2-Phenanthrene/C_2-Anthracene	10.5
1496	206	C_2-Phenanthrene/C_2-Anthracene	10.7
1498	206	C_2-Phenanthrene/C_2-Anthracene	7.4
1510	212	C_2-Dibenzothiophene	9.9
1510	206	C_2-Phenanthrene/C_2-Anthracene	8.2
1518	206	C_2-Phenanthrene/C_2-Anthracene	44.9
1520	212	C_2-Dibenzothiophene	13.9
1527	206	C_2-Phenanthrene/C_2-Anthracene	26.3
1535	206	C_2-Phenanthrene/C_2-Anthracene	15.3
1537	212	C_2-Dibenzothiophene	10.9
1545	206	C_2-Phenanthrene/C_2-Anthracene	7.7
1545	212	C_2-Dibenzothiophene	1.5
1552	202	Fluoranthene	18.1
1569	206	C_2-Phenanthrene/C_2-Anthracene	7.8
1571	226	C_3-Dibenzothiophene	14.4
1592	206	C_2-Phenanthrene/C_2-Anthracene	7.8
1600	226	C_3-Dibenzothiophene	16.0
1618	226	C_3-Dibenzothiophene	28.4
1623	202	Pyrene	30.2
1628	220	C_3-Phenanthrene/C_3-Anthracene	4.9

continued...

Table 6.7.1. Continued.

Scan	m.w.	Compound	ppm
1635	226	C_3-Dibenzothiophene	12.7
1639	220	C_3-Phenanthrene/C_3-Anthracene	4.3
1643	226	C_3-Dibenzothiophene	13.1
1650	220	C_3-Phenanthrene/C_3-Anthracene	6.8
1654	220	C_3-Phenanthrene/C_3-Anthracene	8.6
1659	226	C_3-Dibenzothiophene	2.2
1665	226	C_3-Dibenzothiophene	12.3
1675	226	C_3-Dibenzothiophene	8.8
1682	220	C_3-Phenanthrene/C_3-Anthracene	21.5
1691	220	C_3-Phenanthrene/C_3-Anthracene	52.1
1692	226	C_3-Dibenzothiophene	23.5
1702	226	C_3-Dibenzothiophene	23.5
1707	220	C_3-Phenanthrene/C_3-Anthracene	8.0
1714	220	C_3-Phenanthrene/C_3-Anthracene	20.2
1720	226	C_3-Dibenzothiophene	10.3
1725	216	C_1-Pyrene/C_1-Fluoranthene	5.9
1753	220	C_3-Phenanthrene/C_3-Anthracene	6.2
1761	216	C_1-Pyrene/C_1-Fluoranthene	14.8
1763	220	C_3-Phenanthrene/C_3-Anthracene	10.1
1779	220	C_3-Phenanthrene/C_3-Anthracene	9.6
1794	216	Benzo(a)fluorene	14.9
1799	220	C_3-Phenanthrene/C_3-Anthracene	15.0
1803	234	C_4-Phenanthrene/C_4-Anthracene	5.0
1813	240	C_4-Dibenzothiophene	6.8
1816	234	C_4-Phenanthrene/C_4-Anthracene	9.3
1826	216	C_1-Pyrene/C_1-Fluoranthene	26.8
1831	234	C_4-Phenanthrene/C_4-Anthracene	7.0
1835	216	C_1-Pyrene/C_1-Fluoranthene	17.2
1837	240	C_4-Dibenzothiophene	23.7
1841	234	C_4-Phenanthrene/C_4-Anthracene	5.6
1860	234	C_4-Phenanthrene/C_4-Anthracene	9.3
1877	234	C_4-Phenanthrene/C_4-Anthracene	9.2
1885	234	C_4-Phenanthrene/C_4-Anthracene	7.7
1895	234	Benzonaphthothiophene	24.4
1902	240	C_4-Dibenzothiophene	7.3
1930	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	10.2
1932	234	Benzonaphthothiophene	14.7
1937	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	3.9
1957	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	16.9
1980	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	9.9
1981	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	2.1

continued...

Table 6.7.1. Continued.

Scan	m.w.	Compound	ppm
1989	230	C_2-Pyrene/C_2-Fluoranthene/C_1-Benzofluorene	10.2
1998	230	C_2-Pyrene/C_2-Fluoranthene/C_1-Benzofluorene	6.1
2019	230	C_2-Pyrene/C_2-Fluoranthene/C_1-Benzothiophene	16.6
2028	230	C_2-Pyrene/C_2-Fluoranthene/C_1-Benzofluorene	13.8
2078	240	C_4-Dibenzothiophene	21.8
2074	228	Benzo(a)anthracene	2.0
2085	228	Chrysene/Triphenylene	26.8
2087	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	4.5
2104	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	4.1
2118	248	C_1-Benzonaphthothiophene	11.1
2127	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	9.5
2133	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	5.9
2147	248	C_1-Benzonaphthothiophene	17.0
2149	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	6.9
2162	248	C_1-Benzonaphthothiophene	10.8
2164	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	13.3
2176	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	6.6
2184	248	C_1-Benzonaphthothiophene	32.4
2203	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	8.3
2207	248	C_1-Benzonaphthothiophene	22.2
2220	244	C_3-Pyrene/C_3-Fluoranthene/C_2-Benzofluorene	5.9
2233	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	27.8
2245	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	8.4
2260	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	9.6
2267	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	1.9
2267	262	C_2-Benzonaphthothiophene	11.2
1176	262	C_2-Benzonaphthothiophene	4.3
2278	242	C_1-Benzo(a)anthracene/C_1-Chrysene/C_1-Triphenylene	2.8

continued...

Table 6.7.1. Continued.

Scan	m.w.	Compound	ppm
2283	262	C_2-Benzonaphthothiophene	4.9
2299	262	C_2-Benzonaphthothiophene	9.2
2309	262	C_2-Benzonaphthothiophene	8.2
2315	262	C_2-Benzonaphthothiophene	12.2
2338	262	C_2-Benzonaphthothiophene	28.4
2352	262	C_2-Benzonaphthothiophene	3.7
2359	262	C_2-Benzonaphthothiophene	7.1
2370	262	C_2-Benzonaphthothiophene	6.6
2374	256	C_2-Benzo(a)anthracene/C_3-Chrysene/ C_2-Triphenylene	16.1
2399	256	C_2-Benzoa)anthracene/C_2-Chrysene/ C_2-Triphenylene	19.9
2413	256	C_2-Benzo(a)anthraceneeC$_2$-Chrysene/ C_2-Triphenylene	7.0
2416	276	C_3-Benzonaphthothiophene	10.4
2421	256	C_2-Benzo(a)anthracene/C_2-Chrysene/ C_2-Triphenylene	4.6
2428	256	C_2-Benzo(a)anthracene/C_2-Chrysene/ C_2-Triphenylene	5.8
2440	276	C_3-Benzonaphthothiophene	14.4
2442	256	C_2-Benzo(a)anthracene/C_2-Chrysene/ C_2-Triphenylene	3.9
2447	252	Benzofluoranthene	7.5
2471	276	C_3-Benzonaphthothiophene	24.5
2481	276	C_3-Benzonaphthothiophene	8.0
2493	276	C_3-Benzonaphthothiophene	3.3
2503	276	C_3-Benzonaphthothiophene	5.4
2505	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	2.6
2513	276	C_3-Benzonaphthothiophene	7.3
2513	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	3.1
2520	290	C_4-Benzonaphthothiophene	5.1
2521	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	2.4
2528	252	Benzo(e)pyrene	8.1
2531	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	2.6
2536	276	C_3-Benzonaphthothiophene	4.6
2543	290	C_4-Benzonaphthothiophene	3.9
2543	252	Benzo(a)pyrene	2.6
2546	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	5.3
2554	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	8.1
2570	252	Perylene	7.1

continued...

Table 6.7.1. Concluded.

Scan	m.w.	Compound	ppm
2571	290	C_4-Benzonaphthothiophene	6.0
2577	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	6.9
2594	266	C_1-Benzo(a)anthracene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	4.7
2617	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	3.3
2624	266	C_1-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)-pyrene/Perylene	3.1
2625	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	4.7
2641	290	C_4-Benzonaphthothiophene	4.6
2656	270	C_3-Benzo(a)anthracene/C_3-Chrysene/ C_3-Triphenylene	5.5
2657	266	C_1-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	2.5
2664	266	C_1-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	3.1
2700	266	C_1-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	5.3
2708	266	C_1-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	2.6
2736	280	C_2-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	4.5
2773	290	C_4-Benzonaphthothiophene	4.3
2783	280	C_2-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	3.5
2788	280	C_2-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	1.4
2822	280	C_2-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	1.2
2829	280	C_2-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	3.0
2839	280	C_2-Benzofluoranthene/Benzo(e)-pyrene/Benzo(a)pyrene/Perylene	1.6

Table 6.7.2. Combustion tube oil 159-14, aromatic components, 1983 November.

Scan	M.W.	Compound	ppm
256	128	Naphthalene	38
261	134	Benzothiophene	28
336	148	2-Methylbenzothiophene	18
343	142	2-Methylnaphthalene	59
344	148	C_1-Methylbenzothiophene	29
250	148	C_1-Methylbenzothiophene	14
359	148	C_1-Methylbenzothiophene	57
360	142	1-Methylnaphthalene	47
429	162	C_2-Methylbenzothiophene	3.8
440	162	C_2-Methylbenzothiophene	31
447	156	C_2-Methylnaphthalene	13
449	162	C_2-Methylbenzothiophene	17
463	162	C_2-Methylbenzothiophene	53
463	156	C_2-Methylnaphthalene	33
473	162	C_2-Methylbenzothiophene	72
482	162	C_2-Methylbenzothiophene	27
485	156	C_2-Methylnaphthalene	83
489	162	C_2-Methylbenzothiophene	25
503	156	C_2-Methylnaphthalene	27
522	156	C_2-Methylnaphthalene	11
536	162	C_2-Methylbenzothiophene	6.5
558	154	Dehydroacenaphthylene	6.1
565	176	C_3-Methylbenzothiophene	11
578	176	C_3-Methylbenzothiophene	19
591	170	C_3-Methylnaphthalene	13
592	176	C_3-Methylbenzothiophene	34
597	176	C_3-Methylbenzothiophene	30
598	170	C_3-Methylnaphthalene	7.3
613	176	C_3-Methylbenzothiophene	45
615	170	C_3-Methylnaphthalene	6.2
620	170	C_3-Methylnaphthalene	13
627	170	C_3-Methylnaphthalene	21
638	176	C_3-Methylbenzothiophene	30
648	170	C_3-Methylnaphthalene	32
651	176	C_3-Methylbenzothiophene	9.0
662	176	C_3-Methylbenzothiophene	7.4
672	176	C_3-Methylbenzothiophene	6.1
675	170	C_3-Methylnaphthalene	30
687	176	C_3-Methylbenzothiophene	7.6
696	166	Fluorene	9.1
705	176	C_3-Methylbenzothiophene	9.3
707	176	C_3-Methylbenzothiophene	24
723	168	Propenylnaphthalene	11
735	168	C_1-Biphenyl	5.3
754	182	C_2-Biphenyl	5.9
763	184	C_4-Methylnaphthalene	6.3

continued...

Table 6.7.2. Continued.

Scan	M.W.	Compound	ppm
773	182	C_1-Biphenyl	6.9
787	184	C_4-Methylnaphthalene	4.8
798	184	C_4-Methylnaphthalene	8.1
829	184	C_4-Methylnaphthalene	8.1
853	184	C_4-Methylnaphthalene	6.7
859	184	C_4-Methylnaphthalene	4.8
869	180	C_1-Fluorene	7.5
880	180	C_1-Fluorene	7.8
896	180	C_1-Fluorene	4.2
897	180	C_1-Fluorene	
899	184	C_4-Methylnaphthalene	4.5
920	182	C_2-Biphenyl/C_2-Acenaphthene	4.6
926	196	C_3-Biphenyl/C_3-Acenaphthene	3.9
928	182	C_2-Biphenyl/C_2-Acenaphthene	4.5
932	196	C_3-Biphenyl/C_3-Acenaphthene	3.5
934	196	C_3-Biphenyl/C_3-Acenaphthene	6.6
946	184	Dibenzothiophene	29
952	182	C_2-Biphenyl/C_2-Acenaphthene	5.1
988	178	Phenanthrene	33
1003	178	Anthracene	13.2
1036	208	C_3-Fluorene	5.3
1046	194	C_2-Fluorene	5.4
1055	194	C_2-Fluorene	4.4
1060	194	C_2-Fluorene	4.3
1069	194	C_2-Fluorene	6.2
1083	196	C_3-Biphenyl/C_3-Acenaphthene	5.0
1087	194	C_2-Fluorene	6.8
1100	198	C_1-Dibenzothiophene	29
1112	198	C_1-Dibenzothiophene	3.5
1113	198	C_1-Dibenzothiophene	5.5
1119	196	C_3-Biphenyl/C_3-Acenaphthene	4.8
1130	198	C_1-Dibenzothiophene	19
1142	198	C_1-Dibenzothiophene	14
1154	198	C_1-Dibenzothiophene	9.3
1156	196	C_3-Biphenyl/C_3-Acenaphthene	5.7
1165	198	C_1-Dibenzothiophene	27
1165	198	C_1-Dibenzothiophene	27
1173	192	C_1-Phenanthrene/C_1-Anthracene	33
1177	196	C_3-Biphenyl/C_3-Acenaphthene	3.0
1184	192	C_1-Phenanthrene/C_1-Anthracene	14
1201	192	C_1-Phenanthrene/C_1-Anthracene	37
1204	198	C_1-Dibenzothiophene	6.8
1206	192	C_1-Phenanthrene/C_1-Anthracene	16
1249	212	C_2-Dibenzothiophene	20
1271	212	C_2-Dibenzothiophene	15
1282	212	C_2-Dibenzothiophene	33

continued...

Table 6.7.2. Continued.

Scan	M.W.	Compound	ppm
1318	212	C_2-Dibenzothiophene	84
1330	206	C_2-Phenanthrene/C_2-Anthracene	6.5
1337	212	C_2-Dibenzothiophene	21
1342	206	C_2-Phenanthrene/C_2-Anthracene	9.7
1345	212	C_2-Dibenzothiophene	13
1348	206	C_2-Phenanthrene/C_2-Anthracene	7.8
1359	212	C_2-Dibenzothiophene	7.4
1370	206	C_2-Phenanthrene/C_2-Anthracene	48
1371	206	C_2-Phenanthrene/C_2-Anthracene	5.2
1378	206	C_2-Phenanthrene/C_2-Anthracene	27
1383	226	C_3-Dibenzothiophene	8.6
1387	206	C_2-Phenanthrene/C_2-Anthracene	19
1394	206	C_2-Phenanthrene/C_2-Anthracene	6.2
1400	212	C_2-Dibenzothiophene	18
1402	202	Fluoranthene	15
1417	206	C_2-Phenanthrene/C_2-Anthracene	9.4
1419	226	C_3-Dibenzothiophene	22
1439	206	C_2-Phenanthrene/C_2-Anthracene	12
1445	208	C_3-Fluorene	23
1465	226	C_3-Dibenzothiophene	28
1471	202	Pyrene	30
1490	226	C_3-Dibenzothiophene	20
1507	226	C_3-Dibenzothiophene	14
1511	226	C_3-Dibenzothiophene	16
1521	226	C_3-Dibenzothiophene	6.8
1524	220	C_3-Phenanthrene/C_3-Anthracene	
1528	220	C_3-Phenanthrene/C_3-Anthracene	27
1542	220	C_3-Phenanthrene/C_3-Anthracene	
1543	220	C_3-Phenanthrene/C_3-Anthracene	56
1550	226	C_3-Dibenzothiophene	45
1558	240	C_4-Dibenzothiophene	4.5
1562	220	C_3-Phenanthrene/C_3-Anthracene	34
1568	226	C_3-Dibenzothiophene	18
1575	216	C_1-Pyrene/C_1-Fluoranthene	6.0
1579	220	C_3-Phenanthrene/C_3-Anthracene	8.9
1589	240	C_4-Dibenzothiophene	13
1591	220	C_3-Phenanthrene/C_3-Anthracene	6.9
1599	220	C_3-Phenanthrene/C_3-Anthracene	9.1
1604	240	C_4-Dibenzothiophene	8.9
1611	220	C_3-Phenanthrene/ . C_3-Anthracene	12.3
1626	220	C_3-Phenanthrene/C_3-Anthracene	9.2
1641	216	Benzo(b)fluorene	14
1647	220	C_3-Phenanthrene/C_3-Anthracene	18
1658	240	C_4-Dibenzothiophene	9.6
1675	216	C_1-Pyrene/C_1-Fluoranthene	27

continued...

Table 6.7.2. Continued.

Scan	M.W.	Compound	ppm
1682	216	Benzo(a)fluorene	15
1685	240	C_4-Dibenzothiophene	22
1700	254	C_5-Dibenzothiophene	5.2
1706	240	C_4-Dibenzothiophene	9.8
1714	254	C_5-Dibenzothiophene	5.1
1723	240	C_4-Dibenzothiophene	10.1
1804	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	15
1826	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	8.6
1829	234	Benzonaphthothiophene	12
1835	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	9.9
1843	230	C_2-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	6.4
1858	234	Benzonaphthiophene	13
1863	230	C_1-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	18
1872	230	C_1-Pyrene/C_2-Fluoranthene/ C_1-Benzofluorene	19
1885	254	C_5-Dibenzothiophene	6.5
1909	254	C_5-Dibenzothiophene	5.3
1920	240	C_4-Dibenzothiophene	
1930	228	Chrysene/Triphenylene	27
1946	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5.8
1961	248	C_1-Benzonaphthothiophene	14
1975	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	19
1979	254	C_5-Dibenzothiophene	4.9
1987	248	C_1-Benzonaphthothiophene	23
1994	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	5.2
2008	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	13
2016	254	C_5-Dibenzothiophene	7.6
2019	268	C_6-Dibenzothiophene	4.0
2027	248	C_1-Benzonaphthothiophene	32
2044	244	C_3-Pyrene/C_3-Fluoranthene/ C_2-Benzofluorene	17
2051	248	C_1-Benzonaphthothiophene	22
2076	242	C_1-Chrysene/C_1-Triphenylene	33
2088	242	C_1-Chrysene/C_1-Triphenylene	8.1
2089	242	C_1-Chrysene/C_1-Triphenylene	3.6
2094	268	C_6-Dibenzothiophene	3.8
2101	242	C_1-Chrysene/C_1-Triphenylene	12

continued...

Table 6.7.2. Concluded.

Scan	M.W.	Compound	ppm
2106	262	C_2-Benzonaphthothiophene	14
2121	242	C_1-Chrysene/C_1-Triphenylene	3.9
2124	248	C_2-Benzonaphthothiophene	10
2138	262	C_2-Benzonaphthothiophene	9
2157	262	C_2-Benzonaphthothiophene	22
2182	262	C_2-Benzonaphthothiophene	28
2187	256	C_2-Chrysene/C_2-Triphenylene	3.6
2215	256	C_2-Chrysene/C_2-Triphenylene	17
2239	256	C_2-Chrysene/C_2-Triphenylene	19
2253	256	C_2-Chrysene/C_2-Triphenylene	7.6
2257	276	C_3-Benzonaphthothiophene	9
2261	256	C_2-Chrysene/C_2-Triphenylene	6.1
2268	256	C_2-Chrysene/C_2-Triphenylene	5.1
2270	256	C_2-Chrysene/C_2-Triphenylene	5.2
2280	276	C_3-Benzonaphthothiophene	17
2292	252	Benzo(b)fluorenthene	8.1
2310	276	C_3-Benzonaphthothiophene	34
2320	256	C_2-Chrysene/C_2-Triphenylene	12
2329	276	C_3-Benzonaphthothiophene	4.2
2352	276	C_3-Benzonaphthothiophene	13
2355	290	C_4-Benzonaphthothiophene	5.6
2369	252	Benzo(e)pyrene	9.8
2376	276	C_3-Benzonaphthothiophene	15

Scan	M.W.	Compound	ppm
2379	276	C_3-Benzonaphthothiophene	15
2384	252	Benzo(a)pyrene	4.2
2395	270	C_3-Chrysene/C_3-Triphenylene	9.3
2410	252	Perylene	8.6
2492	270	C_3-Chrysene/C_3-Triphenylene	4.8
2500	266	C_1-Benzofluoranthene/ C_1-Benzo(e)pyrene/ C_1-Benzo(e)pyrene/C_1-Perylene	7.3
2537	266	C_1-Benzofluoranthene/ C_1-Benzo(e)pyrene/ C_1-Benzo(a)pyrene/C_1-Perylene	7.1
2605	290	C_4-Benzonaphthothiophene	9.8
2617	280	C_2-Benzofluoranthene/ C_2-Benzo(e)pyrene/ C_2-Benzo(a)pyrene/C_1-Perylene	6.4
2665	280	C_2-Benzofluoranthene/ C_2-Benzo(e)pyrene/ C_2-Benzo(a)pyrene/C_1-Perylene	8.0