1

The Chemistry of Petroleum Kingdom

Preface : *It is known that crude oil, the basic raw material of refining industries is not only unique but the entire organic chemistry could be studied in it. Crude oil contains almost all known hydrocarbons and non-hydrocarbons. As it is drawn from the earth, it also contains impurities like water, mud and salts during its exploration and transportation.*

The typical nature of crude oil from different sources are different, it is told that as faces of two human being could not be exactly equal though it may be more or less identical, the same is true for crude oil also, the individual oil even from the same well at different time of extraction is differing in the characteristics in terms of chemical composition and physio-chemical behaviour though the basic trend is almost same for each type of crude oil.

In this chapter a brief concept about the chemical composition of the crude oil is given with the objective to give a clear idea to the refiners the inherent nature of the hydrocarbons and its unwanted elements for giving a meaningful conception for refining the typical crude oil of their interest. The physico-chemical nature of the crude oil available in the world are also compiled for the ready reference along with it.

1.0 INTRODUCTION

Crude oil, usually black in colour, is a mixture of hydrocarbon of eight different families for example (1) Paraffins (2) Cyclopentanes (3) Cyclohexanes (4) Cycloheptanes (5) Di-cyclo-paraffins (6) Benzenes (7) Aromatic cycloparaffins (8) Dinecuclear and polyneuclear aromatics with smaller amounts of organic compounds of sulphur, oxygen and nitrogen and still smaller amounts of compounds containing metallic constituents particularly vanadium, nickel iron and copper.

Each of the substances present has its own B.P. and so they can by separated by heating. Lighter molecules coming out first and the heavier ones at higher temperatures. Many hydrocarbons have B.P.s close to those of their neighbours in the series and of some members of other series. So in practice, the oil is divided into portions or fractions that boil within selected temperature ranges. The fractions are then given further treatment such as thermal and catalytic cracking, reforming, alkylation, isomerisation and polymerisation for final use.

That is why there is always a great difference between the compounds of the products which are obtained from crude oil and that of the finished products. The finished products contains compounds not present in the original crude or present in insignificant amounts. It has been estimated that about 60% of modern gasoline consists of molecules not found in original crude oil.

The crude oil will vary also the kinds of hydrocarbons they contain. Some are paraffinic with 75% or more of chain compounds and others napthenic containing 70% or more of saturated ring compounds. They also vary in the amounts of the lowest members of series present as indicated by the temperature at which they begin to boil which vary from 25°C to 200°C.

The purely hydrocarbon contain may be as high as 97% and as low as 50% for a heavy crude oils, of course even crudes with 50% of non-hydrocarbon contents retain most of the hydrocarbon characteristics. The molecules containing one or perhaps two atoms of elements other than carbon and hydrogen.

The purely hydrocarbon is approximately constant from crude to crude even though the amounts of the various hydrocarbon types and the individual isomers may vary. The carbon contents is usually between 83% to 87% and hydrogen content between 11% to 14%, The ratio of carbon to hydrogen increases some what from the low to high mol. wt. fraction this is attributed to an increase in the content of polynuclear aromatics and multi-ring cycloparaffins in these higher boiling fractions.

Both atmospheric and vacuum distillation are adopted in order to separate the compounds present in crude oil into various fractions. In the atmospheric distillation for a typical crude fractions upto 366°C is collected namely:

1. Over head gases, essentially propane and butane.
2. C5-90°C light naphtha.
3. 90°C - 140°C heavy naphtha
4. 140°C - 204°C mineral turpentine oil
5. 140°C - 240°C aviation turbine fuel,
6. 140°C - 271°C Kerosene
7. 271°C - 340°C gas oil
8. 340°C - 366°C jute batching oil

After 366°C the product, reduced crude oil is feed to the vacuum distillation unit for getting lube oil and bitumens.

The various cuts which are obtained both form atmospheric and vacuum distillation unit are given further treatment to met the specification of the Bureau of Indian Standards before use.

Nearly all the hydrocarbons possibly paraffins, cyclopentane, cyclohexane and benzene series are all present in the gasoline fraction, at least in small amounts. In the kerosene and gas oil fractions the complexity is much more greater, but very few of the large number of hydrocarbons probably present have been isolated from fraction of virgin petroleum boiling above 132°C.

1.1. COMPOUNDS OF STRAIGHT RUN GASOLINE

Paraffins aromatics and naphthenes are present in straight run gasoline, olefins are mostly absent. The percentage of those hydrocarbons depend upon the crude oil from which the gasoline is distilled out paraffins base and mixed base crude produces rich in paraffins. The proportion of paraffins in those gasoline fractions is 50% and may be as high as 70%. The intermediate type with a paraffins content of about 50% is also quite common, such gasolines content about 40% naphthenes.

Highly paraffinic gasolines though are common but the gasolines containing 60% or more naphthenes are comparatively rare and rich in aromatics containing more than 20% are also

rare, The 75% of gasoline fractions is composed of 31 hydrocarbons **and 50/- by 8 and** 34% by only **4 and 20/-** by only 2. That is why, there may actually be thousands of hydrocarbons in the fraction, the major part of the material is made up of a rather small amounts of constituents. Approximately 50% of the gasoline is composed of about 12 hydrocarbons only.

1.2. KEROSENE AND GAS OIL FRACTIONS

Kerosene is composed of chiefly hydrocarbons containing about 11 to 13 carbon atoms per molecule. Gas oil is composed chiefly of hydrocarbons with 15 to about 25 carbon atoms per molecule.

The chief constituent of kerosene is aromatic cycloparaffin including tetrahydronaphthelene, Dicycloparaffin is also occurred in kerosene, but in gas oil, dinuclear aromatics tricycloparaffin and trinuclear aromatics are present in appreciable amounts and very minor part is dicycloparaffin.

Both the kerosene and gas oil contains mixed type of hydrocarbons both aromatics and cycloparaffins rings in the same molecule as for example the indanes and tetrahydronaphthlenes with 5 and 6 membered cycloparaffins rings.

The dinuclear aromatics which are present are mostly of the type of naphthelens and its homologues. However at least a smaller amounts of material with two single aromatic rings is present i.e., biphenyl and 3-methyl biphenyl.

Trinuclear aromatic compounds are mainly phenantherene rather than anthracene, However 10 homologues anthracene have been isolated, with the exception of some normal paraffin, this appears to be the highest molecular weight pure hydrocarbon thus isolated from natural petroleum.

1.2.1. Lubricant Fractions

Lubricating oil are comprised principally 25 to 35 or possibly 40 carbon atoms per molecule. In residual stocks hydrocarbons with 50 to 60 and more (upto 80 of 90) carbon atom per molecule may be present.

Normal paraffins are present in very small amount and branched paraffins are also very low. In some of the lube oil fractions paraffins are almost nil, cycloparaffins and aromatics are principal constituents with non hydrocarbon components.

The branched paraffins amount to 15.8 % of the branched paraffins-cycloparaffins portion. Both cyclopentyl and cyclohexyl nuclei are present.

Paraffinic CH_2 groups are contained principally in unsubstituted chain at least four carbon atoms in length. The aromatics which are present are mainly mono, di and trinuclear. But definitely aromatic with or five nuclei per molecule are present in very small amounts.

Dinuclear aromatics are of the naphthelene type while trinuclear aromatics are phenanthrene type predominates than that of anthracene type, but the greater part of the aromatics occur as mixed aromatic cycloparaffin compounds.

A typical fraction mononuclear aromatic portion content is 11% alkylbenzenes. The rest being composed of mixed type components.

The following Table 1.1 shows the typical gas oil and kerosene, the various fractions present by % volume.

Table 1.1.

Sr. No.	*Types of Hydrocarbons*	*vol. % gas oil out*	*vol % Kero out*
1.	Normal paraffins	22	23
2.	Branched paraffins	8	16
3.	Monocyclo paraffins	29	32
4.	Dicyclo paraffins	17	11
5.	Tricyclo paraffins	4	0
6.	Mononuclear aromatics	12	15
7.	Dinuclear aromatics	8	3

1.3. NON-HYDROCARBON CONSTITUENTS

The non-hydrocarbon constituents are usually concentrates in the higher boiling portions of the crude. The molecular weight of non-hydrocarbon complexes is probable near that of the accompanying hydrocarbons. The followings are main constituents:

1. *Nitrogen Compounds.* Nitrogen compounds in crude oil is generally low about 0.85% by weight maximum.

The presence of nitrogen compound in petroleum is responsible for poisoning the cracking catalysts, formation of gums in such products of domestic fuel oil and are classified as basic and non-basic nitrogen compounds.

Both quinolins and pyridines carrying alkyl substituent as well as few pyridines in which the substituents are cyclopentyl or cyclohexyl group isolated as for example.

3, Cyclopentyl pyridine 4, Cyclopentyl pyridine and 2, (2,2,6 trimethyl cyclohexyl) 4, 6-dimethyl pyridine. Isoquinoline and 1, and 3 methyl isoquinolines have been isolated.

For the straight run distillate the distribution of the several types in the nitrogen concentrated is as follows :

Pyridines	43.9 %
Carbazoles	29.5%
Indoles	9.4 %
Pyrolines	8.9 %
Quinolines	8.3 %

2. *Sulphur Compounds.* Proportion of sulphur compounds increases with boiling point except in the case of decomposition when middle fraction may contain more sulphur than the other. But in the usual distribution above 95% of the sulphur or greater is in the gas oil and residual portions. The following sulphur compounds are isolated:

(*i*) Mercaptans (alkane and cyclo) (*ii*) Thiophenes (Aliphatic and aromatic)

(*iii*) Alkane and cyclic sulphides. (*iv*) Ply-sulphides.

In a typical analysis among the 40 sulphur compounds isolated so far the following are their distribution :

17 alkane thiols (Mercaptans) cyclo alkane thiols 14 alkane sulphides and 9 cyclic sulphides.

Mercaptans or thiols are present in the lighter outs i.e., gasolines, naphthas. Among the open chain thiols, primary thiols are associated upto 5 or 6 carbon atoms and secondary thiols upto 12 to 13 carbon atoms and tertiary thiols are very minor components. For cyclic thiols both 5 and 6 membered rings are present.

Among the thiophenes methyl and ethyl substituted alkyl thiophenes and benzothiophenes containing 1,2,3 rings per molecules are present *i.e.*, in the kerosene range the following are the main :

2, 3, 4 trimethyl thiophene.
2, 3, 4, 5 tetra methyl thiophenes and
2, 3 dimethyl thiophene.
2, 3, 4 trimethyl, 5 ethyl thiophene.

The presence of benzothiophenes boiling in the higher range above gasoline is established and 65% of the sulphur compounds are benzothiophenes containing 1,2 and 3 rings per molecule.

Polycyclic benzothiophenes are condensed aromatic thiophene type, also present in the higher distillate products.

A number of bicyclic sulphides those including 2 condensed 5 membered rings i.e., cis-2-thio bicyclo (3,3,0) octane and those with a 5 and 6 membered rings are present i.e., 2 this bicyclo - (4,3,0) nonane. The interesting trycyclin sulphide, thio-adamantane was also isolated.

Polycyclic sulphides with condensed 5 and 6 membered rings in the kerosene range is present.

3. *Oxygen Compounds.* The total oxygen content of petroleum is upto 2 percent. But the resins and asphaltic materials which are separated from the residues and higher boiling fractions have oxygen contents upto 8% by weight.

Very little is known about the structure of higher weight and the lower molecular weight compound are carboxylic acids and phenols with small amounts of esters, anhydrides or lactones of probable aliphatic acids. Information of presence of alcohol and ketones (or possibly aldehydes) in heavy lubricating oil are also there.

Carboxylic acids with less than 8 carbon atoms per molecules are almost entirely aliphatic nature. Monocylic acids begin at C_6 and predominate at C_{14}.

Branched chain acid through C_6 and normal acids through C_9 were isolated. The presence of myristic, palmitic and stearic and arachidic acids in a gas oil is detected.

Among the cyclic acids those with both 5 and 6 membered rings were isolated.

5 membered rings the following are important :

2- methyl cyclopentane carboxylic acid
3- methyl cyclopentane carboxylic acid
3- methyl cyclopentane acetic acid
2, 3 - dimethyl cyclopentyl acetic acid and
1, 2, 2 -trimethyl cyclopentane carboxylic acid

6 membered ring : P - methyl cyclohexane carboxylic and *cis* and *trans* 2, 2, 6 trimethyl cyclohexane carboxyl acids. Acids are present with carboxyl group attached directly to the ring as well as separated by one carbon atom, acids, with 4, 5 and perhaps more rings per molecule are present in the higher boiling fractions.

4. *Metallic Constituents.* The main metallic constituents are nickel vanadium, iron and copper . But Zinc titanium, calcium and magnesium compounds were found in addition to those elements. Vanadium compounds in petroleum exists as porphyrin complexes. Both vanadium and nickel derivatives of prophyrin are also identified.

1.4. STRUCTURE ORIENTED LUMPING

A new method called Structure Oriented Lumping (SOL) for describing the composition, reactions and properties of complex hydrocarbon mixtures has been developed. Structure oriented lumping represents individual hydrocarbon molecules as a vector of incremental

Table 1.2. : Classes of Crude Oils

Classification	*High*								*Low*				
Wax Hydrocarbon type	*Paraffinic*		*Mixed base*	*Naphthenic*		*Intermediate (middle east type)*			*Naphthenic*				
Asphaltenes	*Low*		*Low*	*Low*		*Moderate*			*Low*		*High*		
Source	*Brazil*	*Libya*	*UK*	*Nigeria*	*Assam*	*Iraq*	*Venezuela*	*Iran*	*Australia*	*Nigeria*	*Venezuela*	*Canada*	*Trinidad*
Crude Oil													
Gravity API	39°	35°	38°	35°	31	34	31	31	36	20°	25°	15°	17°
Pour point °F	95	70	60	50	95	5	5	10	< – 70	– 40	< – 30	– 10	– 15
Wax (BP)% wt	28	16	14	11	22	7	8	6.5	0.7	1	2	1.6	1
Light Distillates													
Gasoline (15-149°C)													
Specific gravity 60°	0.711	0.712	0.7305	0.745	0.7635	0.7075	0.721	0.720	0.7365	0.776	0.7205	0.7435	0.743
Octane number	48	50	57	71	70	50	54	58	62	72	60	65	66
Naphtha (95-175°C)													
Paraffins% wt	66	62	42	24	25	66	50	44	35	12	47	31	20
Middle Distillates													
Kerosine (149-232°C)													
Specific gravity 60°F	0.772	0.775	0.792	0.8185	0.8805	0.782	0.795	0.798	0.8205	0.843	0.8075	0.8215	0.829
Smoke point (mm)	39	38	28	21	14	26	25	22	21	20	22	22	17
Gas oil (232-342°C)													
Specific gravity 60°F	0.811	0.8165	0.835	0.8595	0.884	0.8395	0.847	0.852	0.8885	0.895	0.8665	0.8845	0.901
Aniline point °C	85.8	83.6	76.0	68.0	49.8	72.5	71.5	68.3	52.9	51.9	63.6	55.2	42.4
Deisel index	80	76	64	81	35	60	67	64	35	33	46	37	28
Pour point°F	30	26	15	10	–16	0	0	0	–75	< –70	–65	< –70	< –75

Heavy Distillates													
Vacuum gas oil (343-371°C)													
Specific gravity 60°F	0.831	0.835	0.851	0.882	0.912	0.877	0.882	0.888	0.9235	0.927	0.907	0.924	0.9385
Aniline point °C	98.6	94.1	88.9	73.2	64.8	76.5	77.5	73.8	60.0	56.2	66.5	56.6	45.5
Diesel index	82	78	67	50	35	50	50	46	30	29	37	29	22
Pour point °F	85	75	70	65	70	50	50	65	–35	–45	–65	–20	–20
Lubricant distillate (371-525°C)													
Specific gravity 60°F	0.850	0.863	0.872	0.911	0.906	0.9095	0.904	0.919	0.942	0.955	0.930	0.948	0.959
Wax (BP) % wt	47	35	28	26.5	43	12.5	11	13	24	<1	<1	1	0.5
Dewaxed oil viscosity index	90	85	81	25	< -30	70	52	43	–8	–65	40	14	–60
Vaccume Residue above 525°C) (potential bitumen)													
Specific gravity 60°F	0.913	0.945	0.931	0.995	0.975	1.006	0.994	1.019	0.994	1.008	1.011	1.050	1.038
Wax (BP) % wt	34	21	26	15	40	10	11	7	7	4.5	6	3	1.5
Asphaltenes % wt	0.15	<0.5	0.7	0.5	0.5	4.4	6.0	7.3	0.7	0.5	9	18	9

Table 1.3. Nahorkatia Crude Oil Analysis

		Total original crude oil	*Total gases upto C_5*	*Atomospheric distillation*				
				Gasoline	*Naphtha (Ref. feed)*	*Kerosene*	*Gasoil*	*Residue*
TBP range	°C	—	—	C_5—140	110—145	140—250	250—370	>370°C
Yield on crude	% wt,	100	3.00	15.9	5.6	16.7	26.2	39.1
Yield on crude	% vol.	100	—	18.3	6.1	17.2	25.7	35.3
Density d_4^{15}		0.8688	—	0.7506	0.7921	0.8395	0.8924	0.9626
API gravity		31.3	—	56.9	47.05	37.0	27.0	15.5
RVP at 37.8°C	Kg/cm^2	0.36	—	0.27	—	—	—	—
Water content	% Vol.	0.9	—	—	—	—	—	—
Pour point	°C	+30	—	—	—	—	—	5.4
Redwood visocity,								
at 37.8°C		42.4	—	—	—	—	—	—
at 50°C		36.7	—	—	—	—	—	—
Carbon residue conradson,	% wt	1.80	—	—	—	—	0.015	4.9
Ash,	% wt	0.01	—	—	—	—	—	—
Sulphur, Total	% wt	0.248	—	0.0025	—	0.026	0.190	0.55
Wax content (engler Holde)	% wt	10.1	—	—	—	—	—	—
Doctor Test			—	neg.	—	neg	—	—
Copper strip corrosion at 50°C 3 hrs		—	—	la	—	la	la	—
Aromatics	% Vol.	—	—	16	34	39	45	—
Hydrocarbon Naphthenes	% Vol.	—	—	43	38	61	55	—
Paraffins	% Vol.	—	—	41	38	(Saturates)	—	—
Kin. Vis. at 37.8°C	Cs	—	—	—	—	—	4.61	—
Aromatics by sulphonation	% Vol.	—	—	—	—	—	45.0	—
Colou! Saybolt		—	—	—	—	+21	—	—
Flash Point,	°C	—	—	—	—	47.2 (Abel)	140 (PMCC)	236 (PMCC)
Smoke Point,	mm	—	—	—	—	12	—	—
Acidity,	mg KOH/gm	—	—	—	—	—	—	—

Aniline point,	°C	—	—	—	—	33.0	54.0	—
Diesel Index		—	—	—	—	—	34.9	—
Cetane no. clear		—	—	—	—	—	37.4	—
Cetane no. +0.1% Vol. Kerobrisol		—	—	—	—	—	42.0	—
Octane no. (Research) clear		—	—	75.1	—	—	—	—
Octane no. -0.4 ml TEL/lit		—	—	88.4	—	—	—	—
Kin Visc. at 60°C	Cs	—	—	—	—	—	—	81.21
at 98.4°C	Cs	—	—	—	—	—	—	14.46
Ref. Index at 20°C		—	—	—	1.4419	—	—	—

Tabel 1.4: Ankleswar Crude Oil Analysis

		ATMOSPHERIC DISTILLATION								
		Total original crude oil	*Gasolines I*	*II*	*Naphtha (Ref. feed)*	*Kerosene*	*Diesel I*	*Oils II*	*Residues*	*II*
TBP range °C	% wt	—	20—100	20—150	100—150	150—250	240—350	240—370	>360	> 370
Yield on crude	% vol	100	11.9	27.6	15.7	24.2	23.2	26.0	23.2	21.8
Yield on crude		100	13.6	30.1	16.5	24.4	22.1	24.7	20.8	19.6
Density d_4^{15}		0.793	0.694	0.728	0.755	0.787	0.833	0.834	0.880	0.8813
API gravity		46.86	72.34	62.81	55.85	48.22	38.28	38.08	—	28.97
Pour point,	°C	15					0	6	48	48
Kin viscosity at 37.8°C	Cs	1.90					3.40	3.72		
RVP at 38.7°C	Kg/cm^2	0.47	0.85	0.44						
Water content	% V	0.1								
Sediment,	% W	0.16								
Carbon residue conradson	% W	0.44					0.1 (Ram bottom)	0.1 (Ram bottom)	—	2.2
Salt content,	% W	0.001								
	lb/bbl	3.0								
Total sulpur,	% W	0.05				0.005	—	0.025	0.1	—
	PPM	—	2	2	2				**	**
Ref. index at 20°C		—	1.3923	1.4111	1.4211	1.4399	1.4666	1.4669		

Aniline point	°C	—	55.4	51.6	48.3	64.5	77.5	79		
Aromatics,	% V	—	3.0	7.5	12.8	13.5				
Doctors test		—	neg.	neg.	neg.	neg.	neg.	neg.		
Copper corrosin for 3 hrs, at 50°C	—	<la	< la	< la	< la	< la	< la (at 100°C)	(at 100°C)		
Oxidation stability minutes		—	—	> 360						
Butane Content	% W	—	4.8	2.0						
Octane no. (Research) clear		—	—	58						
Octane no. (Research) + 0.4 ml/l TEL		—	—	71.5						
Colour saybolt		—			> +30	+23				
Aromatics	%V	—			12.8					
Hydrocarbon Naphthenes	%V				34.9					
composition Paraffines	% V				52.3					
Acidity total, mg KOH/g		—			0.01	0.2	0.1	0.1		
Flash Point, P & M closed,	°C					52	112	120	202	220
Smoke point		°C					28			
Kin, Viscosity at 20°C	Cs					1.64				
Acidity in-organic **						nil	nil	nil		

		I	II							
Viscosity redwood I at 50°C, Sec.		121	132.7							
Equivalent Kin, Vis at 50°C, Cs		29.2	32.5							
Visc. Redwood I at 93.3 °C, Cs		49	49							
Equi. Kin Visc. at 93.3 °C, Cs		8.8	8.8							
Ash,	% wt	0.07	0.08							
Asphaltenes,	% wt	1.5	—							
Calorific value,	Cal/g	10765	—							
C, %		86.64	—							
H, %		12.82	—							

		I	II							
* Diesel Index		65.7	66.3							
Ash % W		—	0.01							

Table 1.5: Typical Crude Oil Analysis Kuwait Export Crude 31.3° API Gravity

		Atmospheric Distillation								*Vacuum Distillation*		
		Distillates					*Residues*			*Distillate*		*Residue*
	Total original crude oil	*Gas C_1-C_4*	*Gasolines (debutanised)*		*Naphtha ref. feed*	*Kerosine*	*Diesel oils*		*Fuel oils*		*Wax distillate*		*Bitumen (Feedback)*
											Ong.	*De-waxed*	
TBP range °C	—	to 15	15-95	15-149	95-175	149-232	232-343	343-371	> 343	> 371	371-525		> 525
TBP range °F	—	to 60	60-203	60-300	203-347	300-450	450-650	650-700	> 650	> 700	700-977		> 977
Yield on crude % wt	100	1.77	6.05	13.55	11.6	12.25	17.0	4.15	55.45	51.3	21.0	18.7	30.3
Yield on crude % vol	100	2.52	7.85	16.65	13.4	13.65	17.5	4.1	49.8	45.75	19.85	17.5	25.9
Specific gravity 60°F/60°F	0.869	—											1.016
			0.663	0.749	0.749	0.785	0.843	0.885	0.967	0.975	0.917	0.929	
Total sulphur % wt	2.5	—				0.15	1.27	2.41	4.02	4.16	2.86	—	5.00
			0.020	0.049	0.049								
Mercaptan sulphur % wt	—	—					—	—	—	—	—	—	—
			0.015	0.018	0.018	0.006							
H_2S (dissolved) % wt	nil	—	nil	nil	nil	nil	—	—	—	—	—	—	—
Patallins % wt	—	—	87.5	77	67.5	62	—	—	—	—	—	—	
Naphthenes % wt	—	—	11	16	18.5	20	—	—	—	—	—	—	—
Aromatics % wt	—	—	1.5	7	14	18	—	—	—	—	—	—	—
Octane number (Research) clear	—	—	63.5	50	35	—	—	—	—	—	—	—	—
Octane number +2.5 ml TEL/UK gal	—	—	79	67	54	—	—	—	—	—	—	—	—
Smoke point mm	—	—	—	—	—	28	—	—	—	—	—	—	—
Freezing point °C	—	—	—	—	—	54.5	—	—	—	—	—	—	—
Aniline point °F	—	—	—	—	—	60	70	74	—	—	—	—	—
Diesel index	—	—	—	—	—	68	58	47	—	—	—	—	—
Cloud point °F	—	—	—	—	—	10	52	—	—	—	—	—	—
Pour point °F	–25	—	—	—	—	—	5	50	60	70	80	0	—

Wax content (BP)	%wt	5.5	—	—	—	—	trace	ca 5	12.8	9.1	8.7	10.8	—	7.6
Viscosity at 70°F	cs	17.0	—	—	—	—	—	—	—	—	—	—	—	—
100°F	cs	9.6	—	—	—	—	1.15	3.53	9.85	1.150	2.185	47	59.2	233.000
122°F	cs	—	—	—	—	—	1.00	2.79	6.8	480	850	27	—	51.000
140°F	cs	—	—	—	—	—	—	—	—	260	436	18.4	—	17.700
210°F	cs	—	—	—	—	—	—	—	—	44.6	64.6	6.12	6.7	837
Viscosity index		—	—	—	—	—	—	—	—	—	—	—	62	—
Acidity	mg KOH/g	0.15	—	—	—	—	0.02	0.07	0.14	0.17	0.17	0.23	—	0.16
Total nitrogen	ppm	1200	—	—	—	—	—	40	290	—	—	790	—	—
Total ash	% wt	0.006	—	—	—	—	—	—	—	0.011	0.012	—	—	0.02
Vanadium	ppm	27	—	—	—	—	—	—	—	49	53	1	—	88
Nickel	ppm	7	—	—	—	—	—	—	—	13	14	1	—	22
Carbon residue (Con)	% wt	5.2	—	—	—	—	—	—	—	9.3	10.1	—	—	17.4
Asphaltenes	% wt	1.4	—	—	—	—	—	—	—	2.5	2.7	—	—	5.0
Molecular weight	(av)	—	54	82	96	118	150	222	289	550	595	383	—	965
Water	% vol	trace	—	—	—	—	—	—	—	—	—	—	—	—
Salt	lb/1,000 bbl	4	—	—	—	—	—	—	—	—	—	—	—	—
Reid vapuor pressure	lb	av 8	—	8.8	4.9	0.6	—	—	—	—	—	—	—	—
Gas C_1-C_3	% wt	0.45	25	nil	nil	—	—	—	—	—	—	—	—	—
C_4	%wt	1.32	75	nil	nil	—	—	—	—	—	—	—	—	—
C_5	%wt	2.11	nil	35	15.6	—	—	—	—	—	—	—	—	—

Table 1.6: Yield of Distillate in Relation to Crude Gravity and Hydrocarbon Type

Crude oil		*Approximate TBP weight per cent yield of total distillate to 700°F (371°C)*		
API	*SG 60°F*	*Normal**	*High (generally naphthenic†)*	*Low (generally waxy‡)*
10	1.000	18		—
15	0.966	26	Canada 29, Quiriquire 40	—
20	0.934	33	Canada 37, Nigeria and Trinidad 48, Seria 61	—
25	0.904	41	Canada 44, Nigeria and Trinidad 55	Emmilichheim (Germany) 26
30	0.876	49	Assam 60, Nigeria 62, Trinidad 68	Boka (Yugoslavia) 35
35	0.850	58	W. Texas 65 Nigeria 69 Seria 80 Barrow Is. 82	Minas (Sumatra) 42 Sarir (Libya) 48
40	0.825	66	Nigeria 75 Papua 80	Bahia (Brazil) 48 UK 56
45	0.802	75	Nigeria 83	Ohanet (Algeria) 67
50	0.780	83	Nigeria 89	—

* This "normal" relationship applies fairly closely to the majority of crudes, including all those from the Middle East, most of those from Venezuela (except from E. Venezuela) and most of the North African crudes. It also applies to many of the crudes from USA, Canada, Colombia, Europe and Russia.

† All these crudes are naphthanic (or naphthenic/aromatic in the case of West Texas) but the lighter Nigeria, Seria, Panua and Barrow Island crudes also contain appreciable amounts of wax.

‡ Although all these crudes have relatively high wax contents, this alone is not necessarily a criterian of a low yield of distillate.

Table 1.7: Distribution of Sulphur (% weight)

	Zubair		*Gach Saran*	
	Total sulphur	*Mercaptan sulphur*	*Total sulphur*	*Mercaptan sulphur*
Crude	1.95	—	1.58	—
Gasoline	0.016	< 0.001	0.14	0.07
Kerosine	0.057	< 0.001	0.26	0.006
Diesel oil	1.11	< 0.001	1.01	< 0.001
Fuel oil	3.40	—	2.58	—

Table 1.8: Total Sulphur Content Distribution in Typical Light, Medium and Heavy Crudes.

	Middle East			*Africa*			*Venezuela*			*Canada*		
Crude oil gravity *API	40°	31°	25°	44°	37°	27°	43°	30°	16°	40°	25°	7°
Total sulphur % wt												
Crude	0.74	2.50	3.86	0.14	0.14	0.25	0.20	0.96	0.32	0.26	2.37	5.08
Gasoline	0.011	0.025	0.069	0.004	0.007	0.01	0.001	0.004	0.027	0.016	0.084	—
Kerosene	0.040	0.15	0.46	0.011	0.004	0.039	0.001	0.042	0.174	0.030	0.34	0.78
Diesel oil	0.59	1.27	2.11	0.12	0.07	0.17	0.19	0.60	1.14	0.25	1.39	1.79
Residual fuel	1.49	4.02	5.43	0.36	0.23	0.40	0.51	1.60	2.78	0.52	3.39	5.36
Vacuum distillate*	1.23	2.86	3.57	0.33	0.18	0.33	0.47	1.12	2.16	0.44	2.39	3.68
Vacuum residue†	1.82	5.06	6.46	0.44	0.3	0.55	0.73	2.12	3.12	0.66	4.26	6.13

Table 1.9. Wax Content's of Crude and Products — Effect on Pour Point

Wax content	*Very high*			*High*		*Moderate*				*Low*		*Very low*		
Crude	*Brazil*	*Sumatra*	*Libya*	*UK*	*Nigerian*	*Middle East Abu Dabi*	*Middle East Qatar*	*Middle East Iran*	*Middle East Neut Zone*	*Aljeria*	*Venezuela*	*Venezuela*	*Trinidad*	*Venezuela*
Crude oil gravity °API	39.5°	36.5°	35°	38°	35°	39°	42°	34.5°	38.5	44°	36.5	16°	23°	25
Total pour point °F	95	95	75	60	50	10	5	-5	-20	<60	30	-5	< -70	< -30
Crude wax %wt	28	32	22	14	10	8.5	6.5	7	5.5	3.3	4.8	1.8	2.6	2.3
Gas oil pour point °F	30	25	25	15	10	5	10	5	5	5	-5	< -70	< 70	-65
wax %wt	17	15	15.5	5	6	4.5	6.5	7	4.5	3.1	2.2		trace	
Heavy pour point °F	85	75	75	70	60	55	55	55	50	45	35	45	35	65
Gas oil wax %wt	47	42.5	38	27	22	13.5	15.5	14.5	12.5	9.7	7.2	0.3	1	
Fuel oil pour point °F	130	125	115	100	110	85	85	80	75	65	50	(85)	50	45
Residue wax %wt	43	53.5	29	28	24	19	16	12.5	8	9.7	7.2	2.6	2.6	4.2
Lub. oil pour point °F			110		120		90	95		75	95	10	35	-25
Distillate wax % wt	46	45.5	34.5	28	26	18	15	12.5	9.5	9	6.3	0.4	1	1
Short vacuum wax % wt	34	38.5	21	26	20	19	16	12	6	11.5	7.7	3.5	4	6
Residue														
Crude type (paraffinic/Intermediate/ Nepahthenic)	P	P	P	P	N	IP	IP	I	I	I	N	N	N	N

"Viscosity pour point"

Table 1.10: Vanadium and Nickel Contents of Crude Oils

	High vanadium (100-1000 ppm)			*Moderate vanadium (10-15 ppm)*			*Low vanadium (less than 5 ppm)*		
Type of crude (generally)	Heavy naphthenic/asphaltic			Intermediate			Low in asphaltenes, low in sulphur and often waxy. Most light crudes (above ca 37° API)		
Regional distribution	Most West Venezuelan crudes. Some heavy Trinidad crudes Some heavy Russina crudes.			Most Middle-east crudes East Venezuela Medium gravity Trinidad crudes Colombian crudes. California and some other USA Heavier Canadian crudes. Some Russian crudes.			Most African crudes (all algeria, Libya, Sahara). Many USA and Canadian lighter crudes. Most European (France, UK, Austria, Yugoslavia, etc.) Most E. Indies and Australian crudes.		
Typical examples .	West Venezuela			Middle East			Africa and Australia		
Vanadium parts/million on crude	1200	293	127	56	36	27	2.4	0.7	< 0.1
Nickel parts/million on crude	150	24	12	20	11	7	13.2	3.7	1.4
Vanadium/nickel ratio	<-	ca 10	->	<-	ca 3	->	<-	ca 0.1	->
Asphaltenes in crude % wt	12.0	3.8	2.0	6.3	1.0	1.4	0.1	0.2	trace
Sulphur in crude % wt	5.5	2.07	1.41	4.47	1.3	2.5	0.25	0.3	0.05
Gravity in crude API	10°	20°	27°	16°	34°	31°	20°	39°	36°

structural feature. A mixture of hydrocarbons is represented as a set of these vectors, each with an associated weight percent. The vector representation of molecules provides a convenient framework for constructing reaction networks of arbitrary size and complexity, for developing molecules based property correlations and for incorporating existing group contribution methods for the estimation of molecular thermodynamic properties. The SOL approach provides a foundation for molecular-based modelling of all refinery process.

Table 1.11. Crude Oil Character for the Available Crudes in the World

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
Abu Dhabi			
Abu Al Bu Khoosh	0.862	32.6	0.78
Arzanah	0.804	44.4	0.52
Jarn Yaphour	0.836	37.7	0.77
Murban	0.8235	40.2	0.81
Components :			
- Asab	0.820	4.0	0.71
- Bab	0.8145	42.1	0.77
- Bu Hasa	0.8285	39.2	0.85
- Sahil	0.8265	39.6	1.46
- Shah	0.874	30.3	0.11
Thammama Condensate	0.7585	54.9	0.11
Thammama 'C' Condensate	0.7585	54.9	0.13
Thammama 'F' Condensate	0.722	51.7	1.43
Umm Shaif	0.844	36.6701	0.12
Uweinat Condensate	0.7125	39.7	1.03
Zakum Lower	0.826	34.9	1.74
Zakum Upper	0.850		
Dubai			
Dubai Export	0.866	31.8	1.91
Margham Condensate	0.7745	51.1	0.039
Egypt			
Belayim Blend	0.892	27.0	2.25
Geisum	0.9425	18.6	4.34
Gulf of Suez	0.871	30.9	1.63
Ras Budran	0.9075	24.3	2.40
Ras Gharib	0.926	21.2	3.52
Zeit Bay	0.854	34.1	1.44
Iran			
Ardeshir (Aboozar)	0.8965	26.2	2.70
Bahrgansar/Mowruz	0.895	26.6	2.70
Cyrus (Soroosh)	0.941	18.8	3.46
Darius (Darood)	0.8555	33.8	2.54
Fereidoon (Foroozan)	0.872	30.7	2.62
Iranian Light	0.854	34.1	1.42
Iranian Heavy	0.868	31.4	1.70
Rostan/Rakhsh	0.8475	35.5	1.69
Sassan (Salman)	0.8575	33.5	2.20
Sirri	0.871	30.9	2.30

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
Iraq			
Basra Light	0.856	33.7	2.13
Basra Medium	0.876	29.2	3.15
Basra Heavy	0.9085	24.2	3.78
Kirkuk	0.8425	36.4	1.90
North Rumaila	0.856	33.7	1.99
Fao	0.8805	29.1	3.15
Kuwait			
Kuwait Export	0.872	30.7	2.49
Neutral Zone			
Hout	0.961	32.8	1.91
Khafji	0.8865	28.0	2.95
Wafra - Burgan	0.915	23.1	3.22
Wafra - Eocene	0.943	18.5	4.30
Wafra - Ratawi	0.905	24.7	3.85
North Yemen			
North Yemem	0.825	39.9	0.096
Oman			
Oman Export	0.848	35.3	0.95
Qatar			
Qatar Export	0.8225	40.4	1.23
Qatar Marine	0.841	36.7	1.47
Saudi Arabia			
Arab Light	0.8575	33.4	1.78
Arab Medium	0.8835	28.6	2.67
Arab Heavy	0.8885	27.7	2.80
Berri	0.8395	37.0	1.22
Sharjah			
Mubarek	0.8365	37.6	0.59
Sajaa Condensate	0.780	49.8	0.08
South Yemen			
West Ayed	0.857	33.5	0.39
Australia			
Airlie Blend	0.805	44.2	0.019
Component			
- North Herald	0.801	45.0	0.020
- South Pepper	0.809	43.3	0.018
Barrow Island	0.841	36.7	0.049
Blina	0.847	35.5	0.089
Challis	0.825	39.9	0.062
Cooper Basin	0.7875	48.1	0.035

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
Gippsland Blend	0.799	45.5	0.089
Jabiru	0.8155	41.9	0.033
Jackson	0.8145	42.1	0.030
N.W. Shelf Condensate	0.772	51.7	0.015
Saladin	0.7885	47.8	0.018
Surat	0.756	55.5	0.020
Talisman	0.8195	41.1	0.052
Varanus	0.8365	37.6	0.035
Brunei			
Champion	0.904	24.9	0.12
Seria Light	0.8265	39.6	0.058
China			
Daqing	0.8615	32.7	0.10
Shengli (1)	0.9125	23.5	1.06
Shengli (2)	0.902	25.3	0.81
Yizheng	0.8835	28.6	0.72
India			
Bombay High	0.828	39.3	0.12
Indonesia			
Anoa	0.801	45.0	0.018
Ardjuna	0.848	35.3	0.11
Arun Condensate	0.7625	53.9	0.02
Attaka	0.8115	42.9	0.04
Bekapai	0.826	39.7	0.08
Bunju	0.869	31.2	0.10
Cinta	0.870	31.1	0.09
Duri	0.9245	21.5	0.20
Handil	0.8555	33.8	0.07
Ikan Pari	0.791	47.3	0.022
Intan	0.8685	30.0	0.10
Kakap	0.797	45.9	0.018
Katapa	0.7835	49.0	0.029
Lalang	0.830	38.7	0.046
Lirik	0.853	34.3	0.07
Minas	0.8485	35.2	0.08
Ramba	0.836	37.7	0.07
Salawati	0.8185	41.3	0.39
Sembakung	0.8475	35.4	0.08
Tarakan/Sanga Sanga	0.896	26.3	0.12

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
Walio Export	0.8475	35.4	0.68
Widuri	0.858	33.3	0.074
Malasiya			
Bintulu	0.879	29.4	0.11
Bintulu Condensate	0.740	59.6	0.025
Labuan	0.8675	31.5	0.80
Miri Light	0.8655	31.9	0.077
Tapis Blend (1)	0.799	45.5	0.029
Tapis Blend (2)	0.7935	46.7	0.036
Components			
- Bekok	0.7835	49.0	0.02
- Guntong - A	0.8805	45.2	0.032
- Irong Barat	0.866	31.8	0.07
- Kepong	0.7895	47.6	0.02
- Palas - A	0.878	47.7	0.027
- Pulai	0.814	42.2	0.02
- Semangkok - A	0.822	40.5	0.038
- Tabu - A	0.8045	44.3	0.029
- Tapis	0.802	44.8	0.03
- Tinggi	0.790	47.5	0.03
- Tiong	0.7994	45.6	0.02
Tembungo	0.8415	36.6	0.064
Terengganu Condensate	0.7305	62.1	0.016
New Zealand			
Maui Condensate	0.749	57.3	0.01
McKee	0.8305	38.8	0.07
Pakistan			
Mazari	0.811	42.9	0.050
Papau New Guinea			
Hedinia	0.8015	44.9	0.039
Thailand			
Erawan Condensate	0.761	54.3	0.013
Vietnam			
Bach Ho	0.823	40.3	0.033
Dai Hung	0.840	36.9	0.08
Algeria			
Algerian Condensate	0.722	64.2	0.003
Hassi Messaoud	0.8005	45.1	0.12
Saharan Blend	0.798	45.7	0.11

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
Zarziatine Blend	0.807	43.7	0.062
Libya			
Amna (Libyan High Pour)	0.8445	36.0	0.16
Bouri	0.8985	25.9	1.81
Brega	0.824	40.1	0.26
Brega Condensate	0.7125	67.0	0.010
Bu Attifel	0.820	41.0	0.04
Es sider	0.8405	36.8	0.38
Sarir (Libyan Export)	0.8415	36.6	0.14
Libyan Light (Sirtica)	0.819	41.2	0.36
Messla	0.8415	36.6	0.16
Zueitina	0.824	40.1	0.32
Syria			
Souedia	0.9115	23.7	4.00
Syrian Light (1)	0.833	38.3	0.40
Syrian Light (2)	0.842	36.5	0.54
Tunisia			
Ashtart	0.878	29.6	1.01
Essaouia	0.826	39.7	0.30
Europe/Russia			
France			
Vert le Grand	0.858	33.3	0.17
Greece			
Prinos	0.862	32.6	3.01
Itally			
Nidle	0.835	37.9	0.40
North Sea			
Alba	0.936	19.6	1.23
Andrew	0.827	39.5	0.12
Argyll	0.8285	39.2	0.16
Auk	0.837	37.5	0.40
Beatrice	0.8305	38.8	0.06
Beryl	0.835	37.9	0.35
Brae Central	0.8635	32.3	0.78
Brent Blend	0.835	37.9	0.39
Brent Spar	0.821	40.7	0.20
Bruce Condensate	0.7675	52.7	0.025
Crawford	0.857	33.5	0.81

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
Cyrus	0.8505	34.09	0.34
Ekofisk	0.8245	40.3	0.16
Ettrick	0.833	38.3	0.28
Everest Lomond	0.784	57.5	0.025
Flotta Mix	0.847	35.5	1.02
Forties Blend	0.832	38.4	0.34
Components :			
- Balmoral	0.836	37.7	0.31
- Brae North	0.8125	42.5	0.17
- Brae South	0.8405	36.8	0.58
- Buchan	0.8515	34.6	0.84
- Forties	0.842	36.5	0.31
- Heimdal condensate	0.7175	65.6	0.004
- Montrose	0.8295	39.0	0.34
Fulmar	0.823	40.3	0.27
Glamis	0.8115	42.8	0.18
Gorm Blend	0.842	36.5	0.24
Gullfaks	0.8815	28.9	0.44
Gyda	0.8285	39.2	0.10
Helm Blend	0.877	29.8	0.55
Components :			
- Helder	0.9265	21.1	0.66
- Helm	0.949	17.5	0.78
- Hoorn	0.9005	25.5	0.63
- Kotter	0.861	32.8	0.54
- Logger	0.858	33.3	0.45
Lyell	0.8435	36.2	0.34
Maureen	0.845	35.9	0.33
Miller	0.832	38.5	0.41
Nelson	0.8305	38.8	0.21
Ninian Blend	0.8345	38.0	0.31
Oseberg	0.8505	34.8	0.29
Rijn	0.8465	35.6	0.24
Statjord	0.8345	38.0	0.27
Thistle	0.8385	37.2	0.31
Russia			
Romashkino (1)	0.8545	34.0	1.30
Romashkino (2)	0.863	32.4	1.23

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
United Kingdom			
Well 98/7-2	0.822	40.5	0.07
Wytch Farm	0.8245	40.0	0.086
West Africa			
Angola			
Cabinda - Export	0.8705	31.0	0.17
Cabinda - Takula	0.862	32.6	0.11
Palanca	0.83	38.9	0.12
Soyo	0.837	37.5	0.15
Benin			
Seme	0.920	22.2	0.41
Cameroon			
Kole Marine Blend	0.863	32.4	0.35
Lokele	0.9375	19.4	0.43
Mokoko Abana	0.9385	19.2	0.42
Congo			
Djeno	0.8905	27.3	0.30
Gabon			
Gamba	0.870	31.1	0.11
Lucina	0.8315	38.6	0.035
Mandji	0.8725	30.6	1.02
M'Bya	0.8525	34.4	0.080
Oquendjo	0.844	36.1	0.67
Rabi-Kounga	0.853	34.3	0.067
Ivory Coast			
Espoir	0.865	32.0	0.34
Nigeria			
Bonny Light	0.8495	35.0	0.13
Bonyy Medium	0.893	26.9	0.22
Brass River	0.8100	43.1	0.074
Escravos	0.8435	36.2	0.143
Forcados Blend	0.883	28.7	0.19
Pennington	0.8425	36.4	0.074
Qua Iboe	0.846	35.7	0.11
Zaire			
Zaire Export	0.8665	31.7	0.10

Country *Crude Name*	*Crude density at 15°C*	*Crude gravity API*	*Sulphur content % wt*
North America			
United States			
Alaska North Slope	0.8945	26.6	1.09
Bay Marchand (S.L.)	0.8465	35.6	0.22
Grand Isle (S.L.)	0.856	33.7	0.30
W. Texas Intermediate	0.8365	39.6	0.27
South America			
Argentina			
Tierra Del Fuego	0.8080	43.5	0.08
Brazil			
Bahia	0.873	30.5	0.22
Carmopolis	0.9065	23.4	0.41
Linguado	0.873	30.5	0.46
Colombia			
Cano Limon	0.8795	29.3	0.52
Cuba			
Isla	0.9685	14.5	5.80
Ecuador			
Ecuador Export	0.876	29.9	0.95
Payamino	0.901	25.6	0.83
Gautemala			
Rubelsanto	0.8845	28.4	3.26
Maxico			
Isthmus	0.854	34.1	1.33
Maya	0.922	21.9	3.11
VS 28	0.8865	28.0	1.53
Peru			
Loreto	0.869	31.3	0.41
Peruvian Low Cold Test	0.8565	33.6	0.08
Venezuela			
Anaco Wax	0.8255	39.8	0.25
Boscon	0.999	10.1	5.50
Jobo/Morichal	0.9845	12.2	2.8
Lagomedio	0.865	32.0	1.24
Lagotreco	0.8635	32.3	1.14
Lamar	0.831	38.7	0.87
Leona	0.908	24.3	1.53
Mercy	0.959	16.0	2.54
Mesa	0.872	30.7	0.93
Santa Rosa Condensate	0.7745	51.1	0.07
Tia Juana 24	0.907	24.4	1.65
Tia Juana Pesado	0.985	12.1	2.66

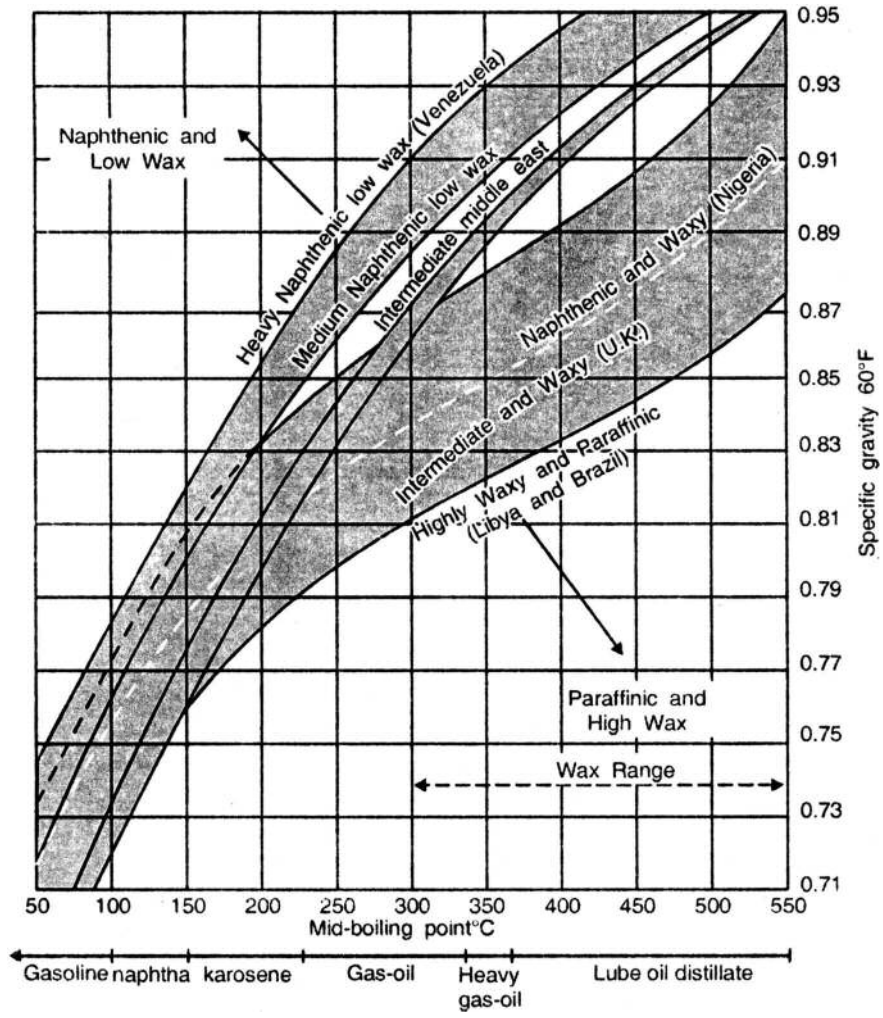

Fig. 1.1. Comparison of crude oils on specific gravity mid boiling point basis.

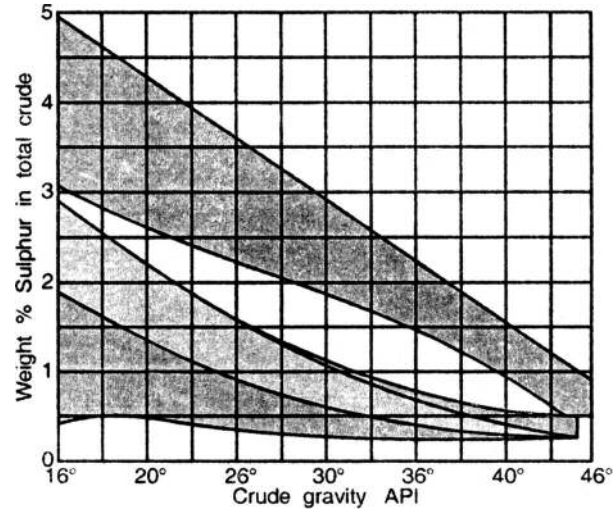

Fig. 1.2. Sulphur content/gravity relationship.

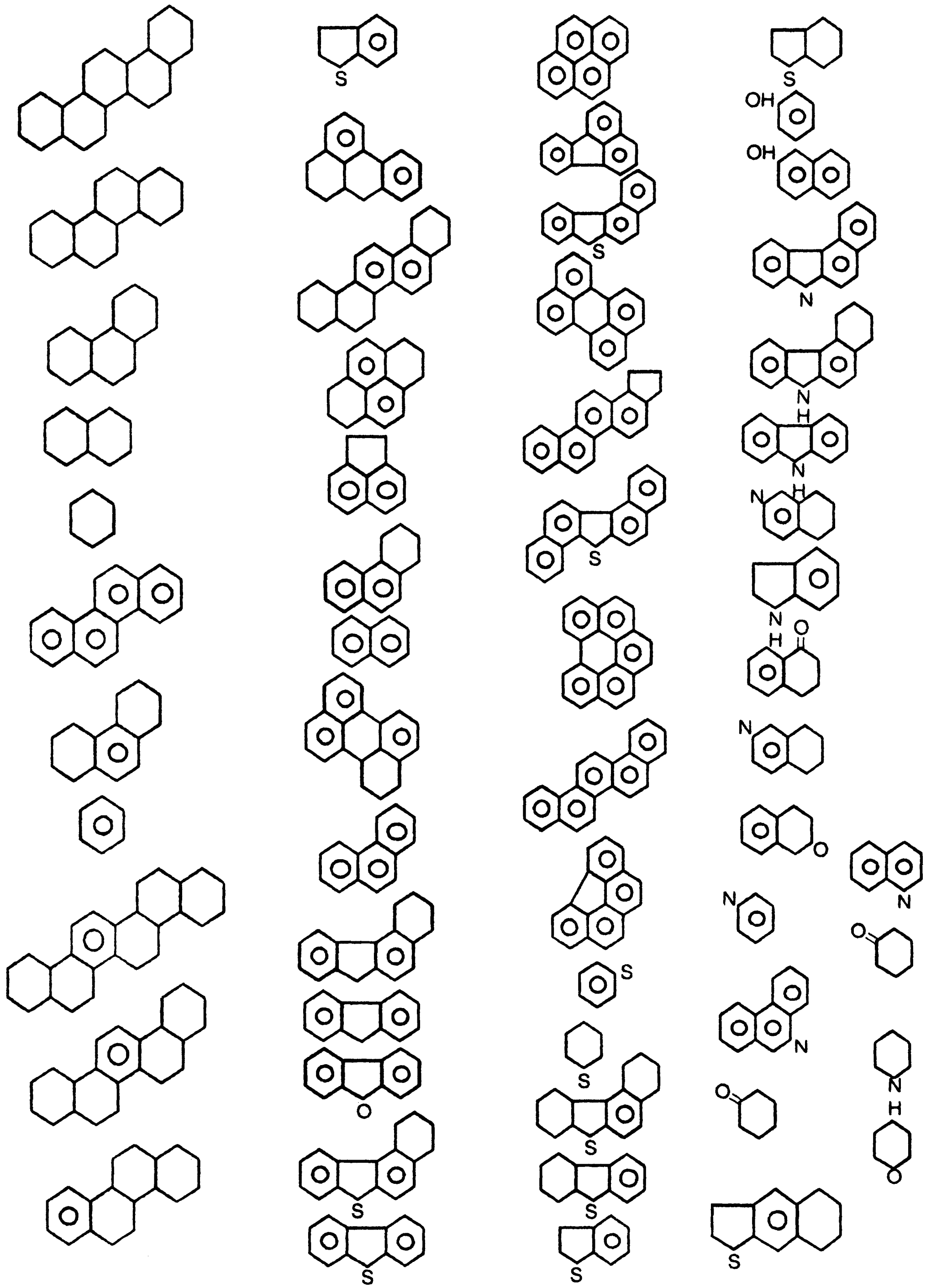

Fig. 1.3. Common structures in crude oils.

References

1. "The Chemistry of Petroleum Hydrocarbons" Brooks, B.T., Kurtz, S.S. Board, C.E. and Schmerling.l.
2. "The Chemistry and Technology of Petroleum" James, G. Speight, Marcel Dekker, N.Y.
3. "Fundamental Aspect of Petroleum Geochemistry" Colombo U.B Naggy, Elsevier 1967
4. "Chemical Engineers Handbook" - Perry J.H.
5. "Pet. Ref. Engineering", A.B.C. Nelson, McGraw Hill
6. Cruid oil Data-book, IOC, New Delhi.
7. 7th World Congress.(1967)
8. "Petroleum Refining Technology and Economics" Marcel Dekker, James H. Gary.
9. "Science of Petroleum" Dunstan Vol-4.
10. "Structure Oriented Lumping", R.J. Ovann and S.B. Jafee Mobil Research and Development Corporation.