THE PREDICTED ENVIRONMENTAL DISTRIBUTION OF SUBSTITUTED BENZENE DERIVATIVES

by

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ABSTRACT

The aim of this study is to calculate environmental equilibrium distributions of substituted benzenes and thus to indicate where each of them goes and what relative concentrations they adopt in the environmental compartments.

With the diversity of chemicals, reasons for predicting their environmental behaviour from their physicochemical properties such as vapor pressure, water solubility and n-octanol-water partition coefficient are obvious. In this study, Mackay's Level I Fugacity Model based on fugacity, a thermodynamic quantity related to chemical potential or activity that characterizes the escaping tendency from a phase, is used for calculations. The fugacity calculations are applied to an evaluative environment, "unit world" consisting of compartments of homogeneous air, soil, water, biota, suspended solids and sediment. Each compartment is assigned a reasonable volume and properties and the equilibrium distributions of those chemicals are calculated using fugacity capacities that are calculated from physical and chemical data and partition coefficients.

When the results are designed to yield priorities for each compartment, it is found that alkyl benzenes except butylbenzene, xylenes, mono- and di-fluorobenzenes, mono- and di-bromobenzenes, mono-, di- tri-chlorobenzenes, iodobenzene for the air compartment,

all phenols, all anilines, acetophenone, benzyl alcohol, butylbenzene, anisole, nitrobenzenes, diiodobenzenes, chloroiodobenzenes, bromoiodobenzenes, bromochlorobenzenes, iodobenzene, dibromobenzenes, tribromobenzenes for the water compartment, diiodobenzenes, tribromobenzenes, hexachlorobenzene, bromoiodobenzenes, chloroiodobenzenes, tetrachlorobenzenes, pentachlorobenzene for the biota, soil, sediment, and suspended solids compartments are priorities.

During this work, good correlations between the mass partitioning of halobenzenes and total molecular surface area, molar volume and π hydrophobic substituent constant are obtained. The mass percentage values calculated by using the correlation equations obtained from this study are in agreement with those calculated through Mackay's Level I approach. Thus these correlations make it possible to calculate the likely equilibrium distribution by using only one property.

ÖZET

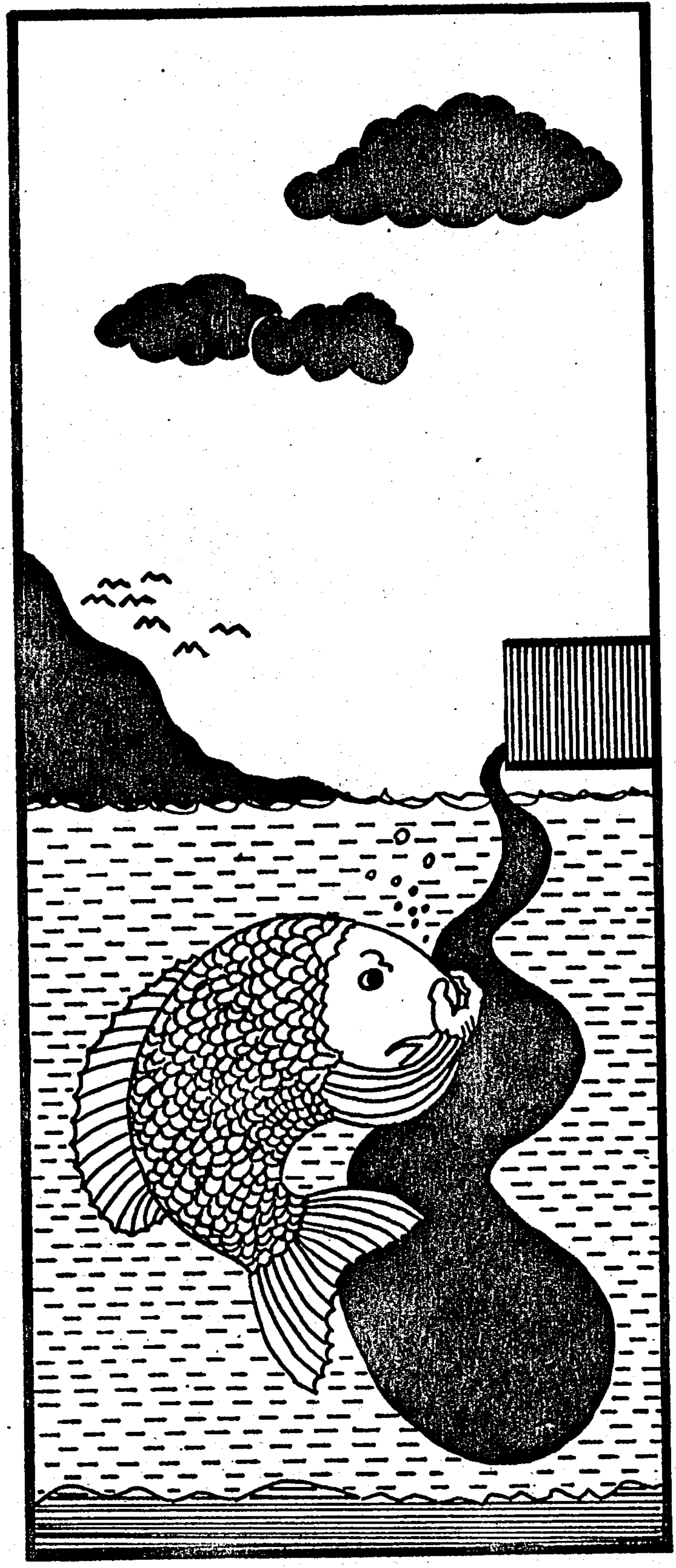
Bu çalışmada substitüye benzenlerin çevredeki denge dağılımlarının hesaplanması ve böylece bu kimyasalların çevrede nereye gideceklerinin, çevrenin çeşitli kompartmanlarında hangi bağıl konsantrasyonlara ulaşacaklarının belirlenmesi amaçlanmıştır.

Çevreye giren maddelerin çok çeşitli olması nedeniyle bunların çevredeki dağılımını sudaki çözünürlüğü, buhar basıncı, normal oktanol su oranı katsayısı gibi fizikokimyasal özellikleri kullanarak hesaplamak giderek önem kazanmaktadır. Bu çalışmada Mackay tarafından geliştirilen maddenin bir fazdan kaçınım yatkınlığı ilkesine dayalı fugasite modelinin birinci aşaması kullanılarak, fizikokimyasal özellikler ve dağılım katsayılarından hesaplanan fugasite kapasiteleri yardımı ile ve fugasite hesaplamaları herbiri belli hacim ve özelliklere sahip homojen hava, su, toprak, biota, asılı madde ve sediment kompartmanlarından oluşan bir teorik birim çevreye uygulanarak substitüye benzenlerin herbir kompartmandaki bağıl miktarları ve bağıl konsantrasyonları hesaplandı.

Elde edilen sonuçlara göre, mono ve dibromobenzenler, mono ve difluorobenzenler, iodobenzen, mono, di, tri-klorobenzenler, ksilenlerin ve butilbenzen dışındaki alkil benzenlerin hava kompartmanı için, tüm fenoller, tüm anilinler, asetofenon, benzil alkol, bütil benzen, anisol, nitrobenzenler, diiodobenzenler, kloroiodobenzenler, bromoiodobenzenler,

bromoklorobenzenler ve tribromobenzenlerin su kompartmanı için, diiodobenzenler, tribromobenzenler, heksaklorobenzen, bromoiodobenzenler, kloroiodobenzenler, tetraklorobenzenler ve pentaklorobenzenin biota toprak, sediment ve asılı madde kompartmanları için öncelikle önem verilmesi gereken kimyasallar olduğu belirlendi.

Ayrıca, bu çalışmada halobenzenlerin her bir kompartmandaki dağılım yüzdeleriyle molekül toplam yüzey alanı, molar hacim ve hidrofobik substituent sabiti arasında bağıntılar bulundu.



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LIST OF SYMBOLS

A	Antoine constant
a	Numerical factor indicating incidence of a given fragment in the structure
B	Antoine constant
c	Antoine constant
C	Concentration
C_a	Equilibrium concentration of chemical in the air phase
C_b	Equilibrium concentration of chemical in the biota phase
C_i	Equilibrium concentration of chemical in each phase
C_o	Equilibrium concentration of chemical in the octanol phase
C_s	Equilibrium concentration of chemical in the soil phase
C_{sd}	Equilibrium concentration of chemical in the sediment phase
C_{ss}	Equilibrium concentration of chemical in the suspended solid phase
C_w	Equilibrium concentration of chemical in the water phase
f	Hydrophobic fragmental constant
f	Fugacity
f_a	Fugacity in air
f_b	Fugacity in biota
f_s	Fugacity in soil
f_{sd}	Fugacity in sediment
f_{ss}	Fugacity in suspended solids
f_w	Fugacity in water
H	Henry's Law constant
K	Partition coefficient

k	Boltzman constant
K_B	Bioconcentration factor
$K_B(f)$	Bioconcentration factor for static terrestrial aquatic ecosystem
$K_B(t)$	Bioconcentration factor for flowing water ecosystem
K_{oc}	Soil organic carbon-water partition coefficient
K_{om}	Soil organic matter-water partition coefficient
K_{ow}	n-Octanol-water partition coefficient
K_p	Soil sorption coefficient
K_{ps}	Soil-water partition coefficient
K_{psd}	Sediment-water partition coefficient
K_{pss}	Suspended solids-water partition coefficient
M	Molecular Weight
M_a	Amount of moles in the air compartment
M_b	Amount of moles in the biota compartment
M_i	Amount of moles in each compartment
M_s	Amount of moles in the soil compartment
M_{sd}	Amount of moles in the sediment compartment
M_{ss}	Amount of moles in the suspended solid compartment
M_T	Total amount of moles
MV	Molar volume
MW	Molecular weight
n	Number of compounds used for correlation
% OC	Percent of organic carbon
P	Vapor pressure
P_1	Vapor pressure at temperature T_1
P_2	Vapor pressure at temperature T_2

P_3	Vapor pressure at temperature T_3
P_a	Mass partitioning of chemical for the air compartment
P_b	Mass partitioning of chemical for the biota compartment
P_i	Mass partitioning of chemical for each compartment
P_s	Mass partitioning of chemical for the soil compartment
P_{sd}	Mass partitioning of chemical for the sediment compartment
P_{ss}	Mass partitioning of chemical for the suspended solids compartment
P_w	Mass partitioning of chemical for the water compartment
P'_a	Equilibrium partitioning of chemical for the air compartment
P'_b	Equilibrium partitioning of chemical for the biota compartmen
P'_i	Equilibrium partitioning of chemical for each compartment
P'_s	Equilibrium partitioning of chemical for the soil compartment
P'_{sd}	Equilibrium partitioning of chemical for the sediment compartment
P'_{ss}	Equilibrium partitioning of chemical for the suspended solids compartment
P'_w	Equilibrium partitioning of chemical for the water compartment
P_T	Total pressure
R	Gas constant
r	Correlation coefficient
RT	Retention time
S	Aqueous solubility
s	Sorbed concentration expressed as volume fraction
S_L	Actual liquid solubility for liquids or subcooled liquid solubility for solids obtained from the actual solid solubility
S_S	Actual solid solubility

T	Absolute temperature
t	Temperature
T_B	Boiling point temperature in °K
T_M	Melting point temperature in °K
t_b	Boiling point temperature
t_m	Melting point temperature
$t_{1/2}$	Fish clearance half life
TSA	Total Surface Area
V	Volume
V_a	Volume of the air compartment
V_b	Volume of the biota compartment
V_i	Volume of each compartment
V_s	Volume of the soil compartment
V_{sd}	Volume of the sediment compartment
V_{ss}	Volume of the suspended solids compartment
V_w	Volume of the water compartment
V_g	Molar volume of gas
V_ℓ	Molar volume of liquid
x	Mole fraction of chemical in the water phase
y	Mole fraction of chemical in the vapor phase
Z	Fugacity capacity
Z_1	Fugacity capacity of chemical for phase 1
Z_2	Fugacity capacity of chemical for phase 2
Z_a	Fugacity capacity of chemical for the air compartment
Z_b	Fugacity capacity of chemical for the bioat compartment
Z_i	Fugacity capacity of chemical for each phase

Z_p	Fugacity capacity of chemical for pure solid and liquid phases
Z_s	Fugacity capacity of chemical for the soil compartment
Z_{sd}	Fugacity capacity of chemical for the sediment compartment
Z_{ss}	Fugacity capacity of chemical for the suspended solids compartment
γ	Activity coefficient
ΔH	The heat absorbed at constant pressure in transferring one mole from gas phase to liquid phase
ΔV	Volume change per mole transferred from gas phase to liquid phase
μ	Chemical potential
μ_1	Chemical potential in phase 1
μ_2	Chemical potential in phase 2
π	Hydrophobic substituent constant
ρ	Density
ρ_a	Density of air
ρ_b	Density of biota
ρ_s	Density of soil
ρ_{sd}	Density of sediment
ρ_{ss}	Density of suspended solids
ρ_w	Density of water
γ_w	Molar volume of water
ϕ	Fugacity coefficient
χ	Sorbed concentration

I. INTRODUCTION

Increasing industrialization and greater dependence on chemical products throughout the world has led to a heightened concern for their effects on the environment. Environmental hazard of a chemical is a function of its toxicity and its exposure. With this in mind there is a need to make an initial assessment of what exposure can be expected from the introduction of a new chemical into an ecosystem. Such assessments need to be made before a new chemical is released into the environment.

The total universe of chemicals [1] which was given by the EPA (Environmental Protection Agency) Toxic Substance Inventory List consists of 40,000 entries in annual production of $1.8\text{x}10^{12}$ kg ($4\text{x}10^{12}$ pounds).

The diversity of the chemicals has created a need for models and programs that can set priorities. Without such a model the task of experimentally making an assessment for each chemical becomes impossible. It will be impossible, for the reason that the man power and resources available are not equal to the task. Furthermore, the need for performing all conceivable tests is not necessary.

By using basic physical and chemical properties of a chemical such as vapor pressure, water solubility, n-octanol-water partition coefficient and molecular weight, the partitioning of that chemical between the major environmental compartments can be quickly assessed. For this purpose, it is necessary to design a model "world" and the volumes and physical properties of its compartments must be selected to mimic as closely as possible a real environment. Thus it is possible to estimate what percentage of chemical will be located in the air, soil, water, biota, suspended solid and sediment compartments. While the results are given in percents, the numbers are not meant to be absolute but are designed to yield a relative rank of importance. From such a distribution further environmental tests if needed, can be designed in a logical and sequential manner. Further tests should be continued until enough is known about degradation, distribution and toxicity of the compound to ensure that the expected environmental concentration resulting from the use is below the no-effect level.

It is hoped that such assessments will bring prior warning of potential impacts of toxic substances. By being aware of the potential environmental problems before they occur, greater precautionary measures can be taken in both manufacture and distribution of the chemical and such action will minimize the effect on the various ecosystems.

In this thesis for benzene and 72 substituted benzenes, the potential concentrations and equilibrium distributions in and between the compartments of an evaluative environment, model world, are calculated by using Mackay's Level I fugacity model. Ranking of them by their potentials to contaminate each compartment is given and correlations between their mass partitioning and other physicochemical properties such as total molecular surface area, molar volume and π-substituent constant related to solubility and n-octanol-water partition coefficient are investigated.

II. REVIEW OF PARAMETERS USED FOR MODELLING AND PREDICTING ENVIRONMENTAL PARTITIONING OF CHEMICALS

2.1 PHYSICOCHEMICAL PROPERTIES

Some progress has been made in using physical and chemical properties to suggest environmental behaviour of chemical contaminants [1-6]. This is an extremely important development since the measurement of physical and chemical properties is considerably easier and less expensive than conducting laboratory or field studies on environmental fate. The main problem is the difficulty in assembling sufficient data obtained by adequate test methods for valid correlation studies. The fundamental physicochemical properties used for modelling and prediction purposes are water solubility, vapor pressure, n-octanol-water partition coefficient and molecular weight.

2.1.1 Water Solubility, S

Water solubility is the saturation concentration of a substance in distilled water. It is a function of temperature.

Water solubility determines the mobility of substances between the environmental compartments air-soil-plant (rainfall) and soil-water (Seepage) [7]. Accordingly, it can influence the wider distribution of a substance (displacement into rivers and oceans). The maximum amount of a chemical in water compartment is governed by the water solubility. Many organic compounds that cause environmental problems have a very low solubility in water. This property, or the inversely proportional high lipophilicity, is most likely a dominating factor in some of their undesirable properties, in particular their tendency to bioaccumulate. In this view the aqueous solubility is an important physicochemical property.

There are only a few numerically reported water solubility data in the chemistry handbooks [8,9]. Gunther et al. reviewed solubility data in the literature and found them to be often contradictory and inaccurate. This is because the solubility of organic compounds in water can easily be influenced by several factors. The presence of electrolytes generally reduces the solubility of non-polar compounds, i.e. the "salting out" effect. Many compounds, particularly hydrocarbons, can exist in colloidal, micellar or particulate form in appreciable quantities, centrifugation and/or filtration reduces the apparent solubility drastically. Water soluble humic substances can act as carriers for lipophilic compounds and surface active organic compounds, many of which occur naturally, increase the colloidal concentration of non-polar compounds, and traces of these surfactants may be responsible for higher solubilities [6,10].

Water solubility data used in this study is obtained from several papers [1,2,6,7,8,11-27].

2.1.2 Vapor Pressure, P

The vapor pressure, P, of a substance is the pressure exerted by the vapor when in equilibrium with the liquid or solid phase [13].

The tendency for an environmental contaminant or pesticide to partition into the atmosphere is determined largely by its vapor pressure. Thus, for assessing the likely environmental behaviour of new and existing chemicals, a knowledge of their vapor pressures is essential. The vapor pressure P (Pa) can be regarded as a measurement of the maximum achievable amount or solubility of the substance in the vapor of air phase, the corresponding concentration being obtained from the gas law as P/RT (mol/m^3) where R is the gas constant 8.314 (J/mol°K) and T is absolute temperature (°K).

The thermodynamic expression of phase equilibrium for a pure substance is given by the Clapeyron equation

$$\frac{dP}{dT} = \frac{\Delta H}{T\Delta V} \qquad (2.1)$$

where P denotes the vapor pressure, T the absolute temperature, ΔH the heat absorbed at constant pressure in transferring one mole from gas phase to liquid (or solid) phase in equilibrium with it and ΔV the volume change per mole transferred.

Equation (2.1) can be simplified by introducing two approximations:

(A) The molar volume of the vapor phase is much greater than that of the liquid (or solid) phase

$$V_g >> V_\ell \tag{2.2}$$

Hence it is possible to neglect V_ℓ and

$$\Delta V = V_g - V_\ell = V_g \tag{2.3}$$

(B) At low pressures it may be assumed that the vapor phase behaves ideally, i.e. according to the equation of state of an ideal gas, so that

$$V_g = RT/P \tag{2.4}$$

On substituting the simplifying relations (2.3) and (2.4) into Eq. (2.1) and rearranging, Clausius-Clapeyron equation is obtained.

$$\frac{1}{P}\,\frac{dP}{dT} = \frac{\Delta H}{RT^2} \tag{2.5}$$

or

$$\frac{d\ln P}{d(1/T)} = -\,\frac{\Delta H}{R} \tag{2.6}$$

or

$$\ln(P_1/P_2) = (\Delta H/R)((1/T_2) - (1/T_1)) \tag{2.7}$$

By integrating (2.6) under the simplifying assumption that

$$\Delta H = \text{constant} \tag{2.8}$$

it is possible to write

$$\log P = A - B/T \tag{2.9}$$

where A and B are constants

$$B = -\Delta H/2.3026R \tag{2.10}$$

Typical vapor pressure characteristics of a substance are illustrated in Figure 2.1.1. The range of environmental temperatures may lie anywhere on this diagram for a given substance, relative to the phase transition points. The solid and liquid vapor pressure lines are highly nonlinear. The Clasius-Clapeyron equation suggest that $d(\ln P)/d(1/T)$ should be fairly constant if ΔH is fairly constant. Figure 2.1.2 shows this plot which is close to linear over small temperature ranges [28]. This relation may be used for interpolation and with caution, for extrapolation in narrow range of temperatures.

The formula [29] to obtain a value of $\log P_2$ for a temperature T_2 from values of $\log P_1$ and $\log P_3$ for temperatures T_1 and T_3 is

$$\log P_2 = \log P_1 + (\log P_3 - \log P_1)(T_2 - T_1)T_3/(T_3 - T_1)T_2 \tag{2.11}$$

where P is the vapor pressure in mm Hg, T is the absolute temperature in °K.

Introduction of a third parameter into Eq. (2.9) gives Antoine Equation [30,31] which represents the behaviour of most substances well over large temperature intervals.

$$\log P = A - B/(t + C) \tag{2.12}$$

where P is the vapor pressure in mm Hg, t is the temperature in °C and

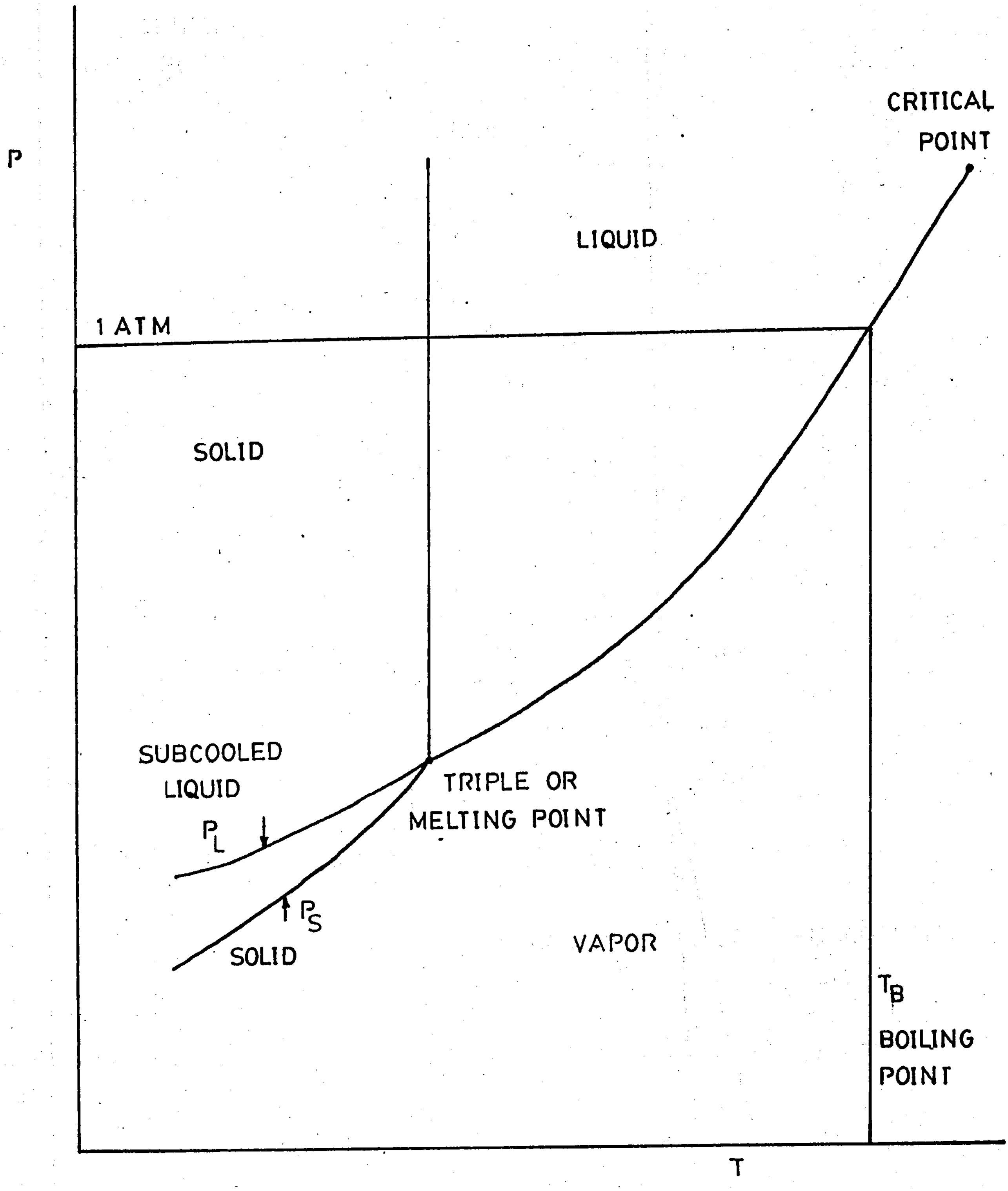


FIGURE 2.1.1. Illustrative plot of vapor pressure (P) vs absolute temperature (T)

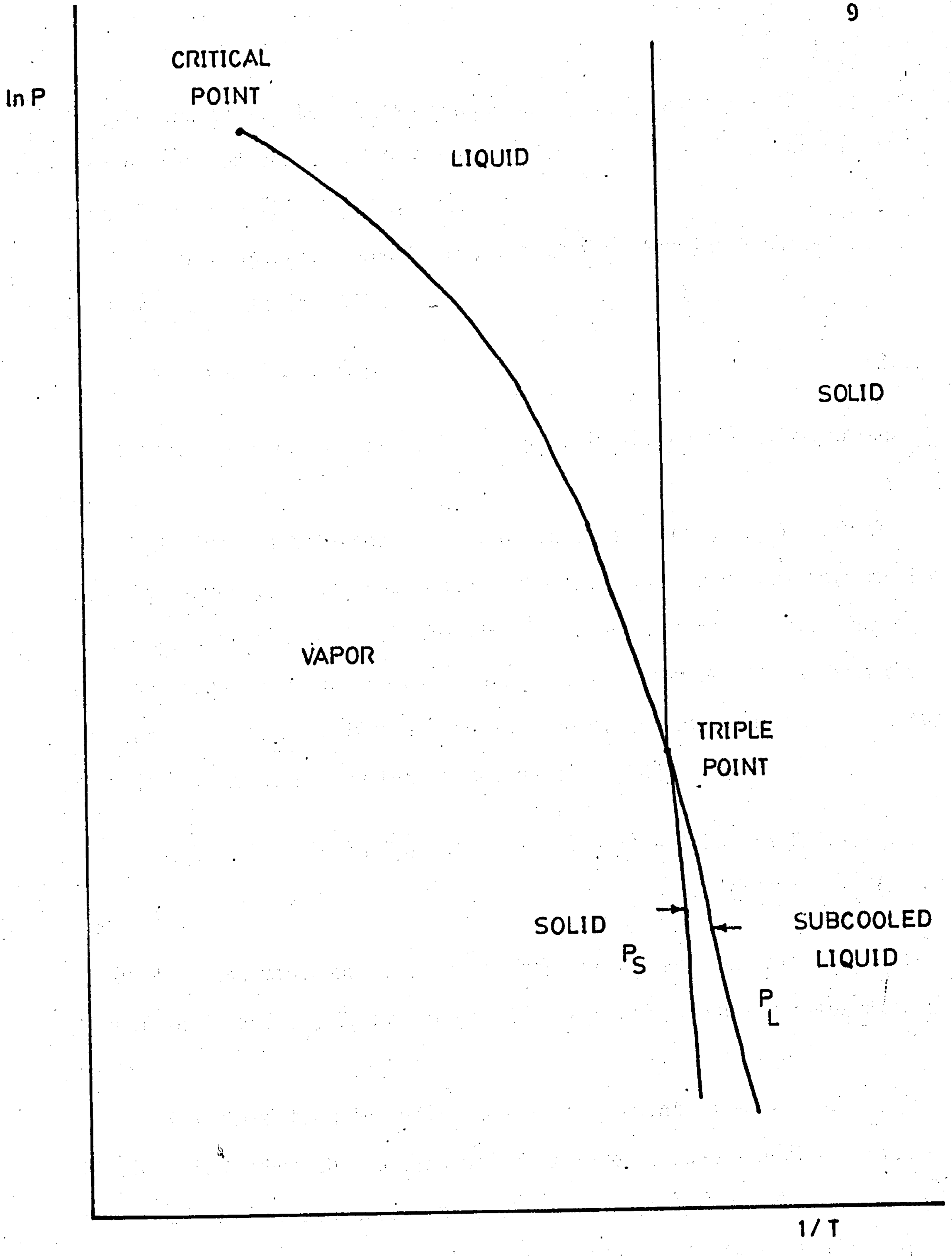


FIGURE 2.1.2. Illustrative plot of ln vapor pressure (lnP) vs reciprocal absolute temperature (1/T)

A, B, C are constants. These constants A, B, C which are characteristics of the substance and the given temperature range, can be taken from literature [30, 31, 32, 33].

When constants B and C are substituted, Antoine Equation can be used in the following form [30]

$$\log P = \frac{-52.23\ B}{T} + C \qquad (2.13)$$

where P is the vapor pressure in mm Hg, T is the absolute temperature in °K.

For some substances of environmental interest, especially for very low vapor pressure substances, the only vapor pressure information that may be available is the boiling point and melting point. One of the equations which can be used to calculate vapor pressures from the boiling and melting points in the absence of experimental vapor pressure data is the Kistiakowsky Linear ΔH Equation [28]

$$\ln P = -(4.4 + \ln T_B)\{1.803((T_B/T) - 1) - 0.803 \ln(T_B/T)\} - 6.8((T_M/T) - 1) \qquad (2.14)$$

where P is the vapor pressure in atmosphere at environmental temperature T in °K and T_B, T_M are the boiling and melting point temperatures in °K.

The third term including the melting point is neglected for liquids, i.e. when the melting point is lower than the environmental temperature. The KLH equation can be applied only to hydrocarbons and halogenated hydrocarbons that boil above 100°C. It is believed that this equation should yield predicted vapor pressures with an average error of only a factor of 1.25. The comparison between the calculated and experimental values have been shown by Mackay et al [28] to be good.

In this study, one of the above-mentioned equations is used according to data available in the literature [1,2,7,9,13,21,22,25,28-34].

2.1.3 n-Octanol-Water Partition Coefficient, K_{ow}

n-Octanol-Water partition coefficient, K_{ow}, is the partition coefficient of the chemical between n-Octanol and water. It has proved to be useful as a means of predicting soil adsorption, biological uptake, lipophilic storage and biomagnification [17,35].

According to the Nerst Law, when a solute partitions at constant temperature between two solvents, which are immiscible or partially miscible, there exists a constant ratio between the solute concentration in the two phases as soon as equilibrium has been attained. A prerequisite for equilibrium is that as many molecules pass through the interphase from phase 1 to phase 2 as from phase 2 to 1. In thermodynamic terms, the equilibrium is characterized by equality of the chemical potentials μ_1 and μ_2, of the solute in the two phases,

$$\mu_1 = \mu_1^\circ + kT \ln C_1 \tag{2.15}$$

$$\mu_2 = \mu_2^\circ + kT \ln C_2 \tag{2.16}$$

if $\mu_1 = \mu_2$ then

$$C_2/C_1 = e^{-(\mu_2^\circ - \mu_1^\circ)/kT} = e^{-\Delta\mu^\circ/kT} = K \tag{2.17}$$

In these equations, C_1 and C_2 represent the equilibrium concentrations of the solute, μ_1 and μ_2 the chemical potentials at these concentrations, μ_1° and μ_2° the chemical potentials at $C_1 = C_2 = 0$, k, the gas constant per mole (Boltzman Constant), T, the absolute temperature (°K) and K, the partition coefficient.

One of the solvents used is always water, and there is a wide selection of organic compounds to choose as the other solvent. The partition coefficient can now be written as

$$K = C_o/C_w \tag{2.18}$$

where C_o and C_w are the equilibrium concentrations of the solute in the organic and aqueous phase, respectively. A solute with high K is regarded as lipophilic and a solute with low K as hydrophilic. As the K scale covers a range of more than 10^{10}, logarithmic K values are usually preferred. This transforms equation (2.18) into (2.19)

$$\log K = \log C_o - \log C_w \tag{2.19}$$

Although various organic solvents have been used, n-octanol having a relatively low water solubility (estimated between 300 and 540 ppm) is considered a good medium for simulating natural fatty structures in plant and animal systems exposed to chemicals [6,10]. When n-octanol and water are used, the partition coefficient is called n-octanol-water partition coefficient and shown by K_{ow}.

Variability in K_{ow} for a given chemical is frequently encountered in the literature. Many factors such as temperature, pH, purity of the solvents, purity of the chemical, volatility of the chemical, mixing time and phase seperation time are all apt to influence the results obtained. The use of gas-liquid chromatography methods for chemicals such as DDT may give high K_{ow} because of the problem of determining low concentrations in water. Radiolabelling techniques may give low K_{ow} values because of trace radioactive impurities that are more water soluble than the chemicals whose K_{ow} are being measured. The latter problem can be minimized by repeated extractions of the octanol layer with water until a constant ratio of activity between the two layers is obtained [6].

K_{ow} values are not available for most chemicals. Thus it is desirable to be able to arrive at values by prediction as an alternative to experimentation.

By analogy with the Hammett Equation, in 1962 Hansch et al proposed to describe lipophilicity as follows

$$\log K(RX)/K(RH) = \rho\pi(X) \tag{2.20}$$

where K(RX) and K(RH) represent the partition coefficients of RX and RH, $\pi(X)$ represents the hydrophobic substituent constant, i.e., the contribution of substituent X to the lipophilicity of structure RH when X replaces an H atom in RH; and the constant ρ reflects the characteristics of the solvent pair used in determining the partition coefficient.

For n-octanol-water system ρ is taken as 1.000 and then Eq. (2.20) can be written as

$$\log K_{ow}(RX)/K_{ow}(RH) = \pi(X) \tag{2.21}$$

It is possible to transform Eq. (2.21) into Eq. (2.22)

$$\log K_{ow}(R' X_1 X_2 \ldots X_n) = \log K_{ow}(R'H_n) + \sum_{1}^{n} \pi(X_n) \qquad (2.22)$$

Then, unknown low K_{ow} values can be calculated by use of the additive constituent characters together with uncertainty units for groups such as CH_2, OH or NH_2, onto known log K_{ow} values of known molecules [6, 35, 36, 37, 10].

In order to obtain information on the π pattern of functional groups attached to a phenyl ring, Fujita et al [36] determined n-octanol water partition coefficients for 203 mono and disubstituted benzenes. From these values the substituent constant π was calculated for 67 functional groups of benzene. The compounds were considered to belong to eight different systems phenyl acetic acid, phenoxyacetic acid, benzoic acid, benzyl alcohol, phenol, aniline, nitrobenzene and benzene. It has been found that π values are relatively constant from one system to another as long as there are no special, steric or electronic interactions of the substituents not contained in the basic reference molecule. Variations in the π values are greatest when two groups with strong mutual interactions are placed together on the aromatic ring, examples are the NO_2-NH_2 and NO_2-OH combinations.

Another method for calculation of log K_{ow} is the hydrophobic fragmental constant (f) approach given by Rekker [37]. It is based on same assumption that the logarithm of partition coefficient can be calculated by summation of hydrophobic fragmental constants, i.e., the lipophylicity contribution of a constituent part of a structure to the total lipophilicity.

$$\log K(RX) = f(R) + f(X) \qquad (2.23)$$

It is possible to convert Eq. (2.23) into Eq. (2.24)

$$\log K(R' X_1 X_2 \ldots X_n) = f(R') + \sum_1^n f(X_n) \qquad (2.24)$$

can also be written as

$$\log K = \sum_1^n a_n f_n \qquad (2.25)$$

In these equations f represents the hydrophobic fragmental constant, the lipophilicity contribution of a constituent part of a structure to the total lipophilicity, and a is a numerical factor indicating incidence of a given fragment in the structure.

Many f values were statistically derived from experimental measurement of n-octanol-water partition coefficients for many compounds having both aliphatic and aromatic structure by Rekker [37].

Although the log K_{ow} values calculated on the basis of f values differ less from the experimental values than those based on π values [37], both methods, in most cases, give figures within the experimental error of determined log K_{ow} values [10]. Log K_{ow} calculations in general are fast and accurate, and the only alternative in the case of partition coefficients of 100,000 or higher ($\log K_{ow} > 5$), since experimental determinations become extremely difficult. For measured values, the range $-5 < \log K_{ow} < 5$ is generally considered to be experimentally accessible with reasonable accuracy [10].

Another rapid and inexpensive method of estimating K_{ow} developed by Veith and Morris by using reverse-phase high pressure liquid chromatography is the linear calibration of the logarithm of retention time with the logarithm of K_{ow} [6].

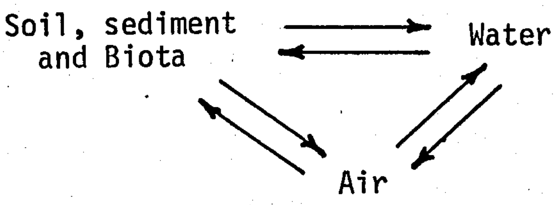
$$\log K_{ow} = 5.106 \log RT - 1.258 \qquad (2.26)$$

where RT represents retention time, K_{ow} represents n-octanol-water partition coefficient.

Most of the log K_{ow} values used in this study are calculated again from experimentally determined π values given by Fujita et al [36]. Only a few of them are calculated by using hydrophobic fragmental constants given by Rekker [37]. Others are taken from literature [6,7,11, 16-20,22,23,26,35,37,38].

2.2 ENVIRONMENTAL PARTITION COEFFICIENTS

All chemicals entering the environment are continually being transported and redistributed between the solid, liquid and gaseous phases of the environment, as illustrated in the following diagram.



In most instances transport of chemicals from soil, sediment, suspended solids and biota to the air and vice versa takes place through water, because these solids are almost always sheathed with water. The rate of transport of the chemicals between the phases depends on the concentrations of the chemicals and their equilibrium partition coefficients between these phases. A substance when at equilibrium adopts different concentrations in air, soil, water, suspended solids and

and sediment compartments. The ratio of these concentrations are given by corresponding partition coefficients. For each substance or solute a partition coefficient can be defined for each pair of environmental compartments.

2.2.1 Henry's Law Constant, H

The air-water partition coefficient is the ratio of concentrations between air and water.

$$H = C_a/C_w \tag{2.27}$$

where C_a represents concentration in air, C_w represents concentration in water and H Henry's Law Constant.

The air-water partition coefficient can be expressed in various forms the most convenient being Henry's Law constant, H in [Pa.m^3]/mol which is the ratio of partial pressure in the atmosphere P in Pa to concentration in water C in mol/m^3.

Henry's Law expresses the proportionality between the concentration of a gas dissolved in a solvent and its partial pressure. In equation form, Henry's law is

$$P = HC \tag{2.28}$$

where P is the partial pressure of the gas, C is the concentration of the dissolved gas, and H is Henry's law constant. Henry's law represents a limiting behaviour for any gas solvent system as its partial pressure approaches to zero.

Typically, Henry's law is no longer valid when partial pressure exceed 5-10 atm and/or when the dissolved concentrations exceed 3 mol%. Henry's law constant is a function of temperature only for a particular gas-solvent system. However, each gas-solvent system has a unique H value.

For prediction and modelling purposes a knowledge of Henry's law constant is essential. Henry's law constants are usually determined by measuring the equilibrium partial pressure and dissolved concentration of the gas and then calculating the ratio of these two quantities. For most environmental contaminants, the aqueous solubilities and vapor pressures of pure substances are very low. Consequently, Henry's law is valid up to dissolved concentrations equal to the aqueous solubility and to partial pressures equal to the vapor pressure of the pure substance. The validity of Henry's law at these partial pressures and aqueous concentrations makes it possible to derive the H's by calculating the ratio of the vapor pressure of the pure compound to its aqueous solubility [39,40]

$$H = P/S \tag{2.29}$$

where P is the vapor pressure of the pure compound in units of Pa and S is the aqueous solubility of the pure compound in units of mol/m^3 and H is the Henry's law constant in units of Pa m^3/mol.

Compounds of high H tend to partition predominantly into the atmosphere and the rate at which they evaporate from water is usually controlled by the water phase mass transport resistance. For substances of low H, partitioning is predominantly into the water, and the evaporation rate tends to be controlled by the resistance in the air phase, where the concentration is lower [28].

2.2.2 Soil (or Sediment) Water Partition Coefficient, K_p

Soil (or sediment) water partition coefficient, K_p is the ratio of the concentrations of chemical between soil (or sediment) and water [1,5]

$$K_p = C_s/C_w \tag{2.30}$$

where C_s is the concentration of chemical in soil, C_w is the concentration of chemical in water and K_p is the soil-water partition coefficient.

Sorption coefficients are relatively constant at low concentrations of chemical in water but tend to decrease as the concentration of the chemical in the water is increased especially for chemicals with high water solubilities.

Sorption is known to be an important factor in the determination of the fate of hydrophobic molecules in a water-sediment or water-soil system.

Various types of intermolecular interactions can be involved in sorption, including Van der Waals - London interactions. hydrophobic bonding and water structure, hydrogen bonding, charge transfer, ligand exchange, ion exchange, direct and induced ion-dipole and dipole-dipole interactions, magnetic interactions and chemisorption [6]. Despite the tremendous complexity of sorption process in soil, there is a remarkably good relationship between the organic matter of soil and their capacity to sorb most organic chemicals, in particular non-ionic organic chemicals [6,41-43]. It is suggested that organic chemicals dissolve in the oily constituents of soil organic matter.

Soil organic matter consists of non-humic substances such as carbohydrates, proteins, fats, waxes, resins, pigments and low molecular weight compounds physically associated with humic acids. Thus some variation in the sorption characteristics of organic matter from different soils can be expected. It is possible to convert percent of organic matter into percent of organic carbon by dividing by 1.74 [6]. Expression sorption of chemicals on a soil organic carbon basis rather than on a total soil basis will eliminate much of the variation in sorption coefficients ordinarily encountered from soil to soil. Referencing sorption to organic carbon gives a partition coefficient to organic carbon, K_{oc}, which is highly sediment and soil independent [42].

The soil organic carbon sorption coefficient, K_{oc}, is the concentration of chemical sorbed by the soil expressed on a soil organic carbon basis divided by the concentration of chemical in the water [6]. The soil sorption coefficient, K_p, is the soil organic carbon sorption coefficient, K_{oc}, multiplied by the percent of organic carbon in the soil [5]. The organic carbon contents are given as 2% for soil, and 4% for sediment and suspended solids [3].

Thus, a 20-30 fold variation in K_p is reduced to less than a two fold variation in K_{oc} by referencing sorption to organic carbon [42]. Greater variability in sorption coefficients expressed on the basis of the organic carbon content of soil can be expected for ionic organic chemicals than for nonionic organic chemicals [6]. Nonionics probably interact with the nonionic portions of the soil organic matter surfaces, which are probably not significantly influenced by the pH of the soil. However, carboxylic acids in ionic form will not be sorbed and may even be repelled from the soil surfaces at high pH values simply because of the negative charge on the soil organic matter surfaces. As the pH of the soil is lowered, the amount of unionized matter sarface and unionized compound increase. Sorption increases simply because of the compound behaves more and more like a neutral molecule.

Residual variation in sorption expressed on the basis of organic carbon is caused by the inherent differences between soils in the sorption characteristics of its organic matter, the impact of other soil properties and soil constituents.

Variations in the sorption coefficients obtained can also be expected as a result of differences in the methodology used to measure sorption.

One factor influencing sorption coefficients is incubation time. Sorption does not reach equilibrium in a short period of time. These appears to be an immediate rapid sorption followed by slow continued sorption over along period of time. Presumably initial sorption is a surface phenomenon followed by a slow migration of the chemical into the organic matter matrix.

Sorption coefficients can also be influenced by the incubation temperature. An increase in solubility with increasing temperature results in a reduction of the amount sorbed [17].

In addition, the ratio of soil to water and the presence of salts or other possible interfering materials influence the sorption coefficients.

K_{oc}'s can be estimated from the measured solute physical properties, namely n-octanol water partition coefficient and solubility. For the available literature K_{oc} data, the estimates derived from n-octanol-water partition coefficients are within the range of measurement variation, attributable to measurement error or reasonable differences in sediment soil sorption [6,41-43].

Soil sorption coefficients based on the organic carbon content of soil, K_{oc}, represent the best way currently available for comparing the sorption characteristics of chemicals. They also represent the most useful measure of comparative leachability in soil.

2.2.3 Bioconcentration Factor, K_B

The bioconcentration factor used in this study can be defined as the concentration of a chemical in aquatic biota divided by the concentration in water [1,6].

$$K_B = C_b/C_w \qquad (2.31)$$

where C_b is the concentration of chemical in biota, C_w is the concentration of chemical in water, K_B is the bioconcentration factor.

The ability of some chemicals to move through the food chain resulting in higher and higher concentrations at each trophic level has been termed "ecological magnification", "bioaccumulation" or "biomagnification" [35]. From the environmental point of view, this phenomenon becomes important when the acute toxicity of the chemical is low and the physiological effects go unnoticed until the chronic effects become evident. Because of insidious nature of the bioconcentration effect, by the time chronic effects are noted, corrective action such as terminating the addition of the chemical to the ecosystem, may not take hold soon enough to alleviate the situation before irreparable damage has been done. For this reason prior knowledge of the bioconcentration potential of new or existing chemicals is desired.

Bioconcentration potential of a chemical is a measure or indicator of the extent to which it may accumulate in aquatic organisms [44]. The actual bioconcentration behaviour of a chemical in an aquatic environment is determined by its bioconcentration potential and by properties of the organisms present in that environment, such as lipid content and capability for metabolizing the substance. Ideally, bioconcentration potential should enable the estimation of a range for maximum bioconcentration, placing upper bounds on the estimated degree to which a chemical may be accumulated in any kind of aquatic organism. The octanol-water partition coefficient has proven to be useful as a measure of bioconcentration potential. It can be assumed that a chemical which does not undergo ready metabolic transformation may express its potential for bioaccumulation though to a different degree, in many species, provided that it is present in the ambient environment for a sufficiently long period of time. In the presence of a metabolic elimination mechanism, the estimates of bioconcentration potential based on lipophilicity may be far too high if the rate of metabolic degradation is rapid [44,45].

The potential of a chemical to bioaccumulate in aquatic organisms can be determined by measuring the bioconcentration factor. Three principal test methods are commonly used for measurement of bioconcentration factors [6].

(A) Exposure of fish in an aquarium to flowing water treated with chemical

(B) A model ecosystem containing plant and/or animal organisms

(C) A terrestial-aquatic model ecosystem containing soil and animal and plant organisms.

The actual bioconcentration factor obtained for a compound is influenced by many factors such as those that influence stability and solubility, particularly in water [6,10].

When a hydrophobic compound is easily metabolized or degraded in water, the tendency to bioconcentrate is offset by a rapid rate of degradation and significant levels of residues do not occur in biota. However the bioconcentration of potentially hazardous metabolites itself be of concern.

Absorption through gills and intestines may be prevented above a certain molecular size or molecular weight of chemical. 600 g/g mole was reported by Zitko as an upper limit in molecular weights of compounds that can be taken up by fish [10].

Since chemicals tend to bioconcentrate in fatty portions of tissues, bioconcentration is directly related, and the rate of clearance inversely related to the lipid content of organism. Lipid content of some aquatic organisms is reported as follows [6]. Atlantic herring 11.3 percent, carp 4.2 percent, freshwater catfish 3.1 percent, yellow perch 0.9 percent, salmon (various species) 3.7 percent to 15.6 percent, book trout 2.1 percent, rainbow trout 11.4 percent, shrimp 0.8 percent, algae 2.32 percent, Daphnia 1.28 percent, mosquito Larvae 1.46 percent, snails 1.6 percent, Gambusia fish 6.15 percent. Lipid content of trout distributed in various tissues as follows. Viscera 92.8 percent, gill 9.7 percent, muscle 2.7 percent, stomach 6.5 percent and liver 3.5 percent. Chemical residues in the tissues are directly proportional to the fat content of these respective tissues. Surprisingly, although lipid content of algae is less than that of fish, algae is apt to give higher bioconcentration factor than fish. This is because it has a high surface to volume ratio compared with large organisms [6].

Bioconcentration factors are directly proportional to n-octanol-water partition coefficients of chemicals when the n-octanol-water partition coefficients are below 10^6, but not when the partition coefficients are above 10^6. This is probably because movements of chemicals in organisms are extremely limited when partition coefficients are above 10^6 [46]. Optimal partition coefficient range at which substances can move most freely in organisms is below 10^4 [46].

Stable chemicals having low water solubilities and high n-octanol-water partition coefficients take the longest time to reach maximum residues in organisms, perhaps several weeks or months. This delay is a reflection of the slow distribution of the compound throughout the organism. Slowness of internal distribution also can be correlated directly with the size of the organism. The time required to reach maximum residues is directly proportional to the size of the organism. Therefore the time necessary to reach the maximum residue concentration in organisms seems to vary greatly for chemicals and species [6].

2.3 CORRELATIONS BETWEEN PARAMETERS

Correlations between parameters are useful as they serve not only as an indication of the interrelationship between them but also as a convenient means to predict a reasonable value for each parameter from known values of every other parameter.

2.3.1 Correlation Between Water Solubility, S, and n-Octanol-Water Partition Coefficient, K_{ow}

Several years ago, the existence of an inverse relationship between n-octanol-water partition coefficient and aqueous solubility was first shown by Hansch and coworkers [10,17] for several classes of relatively low molecular weight organic liquids whose aqueous solubilities generally fall in the high ppm (mg/l) range.

$$\log(1/S) = 1.214 \log K_{ow} - 0.850 \qquad (2.32)$$

S = molal solubility

In the report of Hansch et al, however most partition coefficients of the organic liquids were assessed from the π constants of the substituents in relation to some parent compounds since the experimental values were not determined.

Later, Chiou et al [17] compared K_{ow} ranging over six orders of magnitude with S ranging over more than eight orders of magnitude for 34 chemicals including aliphatic and aromatic hydrocarbons, aromatic acids, organochlorine and organophosphate pesticides and polychlorinated biphenyls. An empirical equation was derived to allow the assessment of n-octanol-water partition coefficient, K_{ow}, from water solubility, S, with a predicted error of less than one order of magnitude

$$\log K_{ow} = 5.00 - 0.670 \log S \tag{2.33}$$

$S = \mu mol/l, \quad n = 34, \quad r = -0.97$

where K_{ow} is the n-octanol-water partition coefficient, S is the aqueous solubility in units of μmol/l, n is the number of compounds used for correlation, r is the correlation coefficient of the equation.

Utilizing data gleaned from literature for 90 organic chemicals having K_{ow}'s ranging from 10^{-4} to 3.7×10^{6} and S's ranging from 10^{-4} ppm to 2.1×10^{6} ppm, Keenaga and Goring [6] studied the relationship between water solubility and n-octanol-water partition coefficient and obtained two regression equations

$$\log S = 4.184 - 0.922 \log K_{ow} \tag{2.34}$$

$S = ppm, \quad n = 90, \quad r = -0.86$

$$\log K_{ow} = 4.158 - 0.800 \log S \tag{2.35}$$

$S = ppm, \quad n = 90, \quad r = -0.86$

Yalkowsky and Valvani [47] correlated water solubility and n-octanol-water partition coefficient for 31 polycyclic aromatic hydrocarbons and indan by the following equation.

$$\log S = -0.88 \log K_{ow} - 0.001\ t_m - 0.012 \qquad (2.36)$$

$S = \text{mol/l}, \quad t_m = °C, \quad n = 32, \quad r = -0.9895$

For liquid solutes, 25°C is used instead of the melting point.

In another study by Yalkowsky et al [16], the dependence of aqueous solubility of 35 halobenzenes on melting point and n-octanol-water partition coefficient was given by

$$\log S = -0.0095\ t_m - 0.9874 \log K_{ow} + 0.7178 \qquad (2.37)$$

$S = \text{mol/l}, \quad t_m = °C, \quad n = 35, \quad r = -0.995$

Banargee et al [23] measured the aqueous solubilities and n-octanol-water partition coefficients of a number of organic compounds which are members of the group of 65 Consent Decree Chemicals for which the U.S. EPA is currently recommending water quality criteria, and a correlation derived from these data very similar to that obtained by Chiou et al [17] (Eq. 1.33).

$$\log K_{ow} = 5.2 - 0.68\ S \qquad (2.38)$$

$S = \mu\text{mol/l}, \quad n = 27, \quad r = -0.54$

During their study Banargee et al noticed that the correlation between these two parameters might be in valid for high melting solids and then, by the treatment of the data by Yalkowsky and Valvani's procedure they greatly improved the generality of the correlation and obtained the equation appropriate to their data.

$$\log K_{ow} = 6.5 - 0.89 \log S - 0.015\ t_m \qquad (2.39)$$

$S = \mu mol/l$, $t_m = °C$, $n = 27$, $r = -0.96$

For liquid solutes 25°C is used instead of melting point.

Mackay et al [19] developed a correlation between melting point, solubility and n-octanol-water partition coefficient based on an examination of the underlying physical chemical equations governing solubility and partitioning.

$$\ln K_{ow} = 7.494 - \ln S \qquad \text{for liquids} \qquad (2.40)$$

$$\ln K_{ow} = 7.494 - \ln S + 6.79(1 - T_m/T) \qquad \text{for solids} \qquad (2.41)$$

$S = mol/m^3$, $T_m = °K$, $T = 298°K$

The differing treatment of solids and liquids arised from the fact that solids had lower solubilities than their subcooled liquids, the ratio of solubilities being the fugacity ratio or the ratio of the solid and subcooled liquid vapor pressures. From Yalkowsky's estimate of the entropy of fusion this ratio could be expressed as $\exp(-6.79(1-T_m/T))$ or $10^{-2.95(1-T_m/T)}$.

Mackay's correlation between melting point, solubility and n-octanol-water partition coefficient was satisfactory for a wide range of hydrophobic compounds but it was not applicable to organic acids. When applied to very high molecular weight (> 290) compounds, the correlation was less satisfactory.

Aqueous solubility and n-octanol-water partition coefficient have been widely used to correlate environmental partitioning phenomena such as bioconcentration and sorption. Therefore, data for both water solubility and n-octanol-water partition coefficient are regarded as essential in any assessment or prediction of environmental fate of chemical substances. The partition coefficients of many compounds of environmental significance are not always available despite a recent extensive compilation. Assessment of partition coefficient from a more readily avaliable physical parameter water solubility would be useful. The water solubility estimates can be useful in assessing whether or not a determined value is reasonable. They can also be helpful in the design of solubility experiments.

2.3.2 Correlation Between Soil Organic Carbon-Water Partition Coefficient, K_{oc}, and n-Octanol-Water Partition Coefficient, K_{ow}

Soil-water partition coefficient, K_p, estimation for hydrophobic organics can be reduced to estimation of soil organic carbon-water partition coefficient, K_{oc}, which when combined with organic carbon content of the soil or sediment, can yield a good estimate of the soil-water partition coefficient, K_p.

The soil-water partition coefficient K_p is K_{oc} multiplied by the percent of organic carbon in soil.

$$K_p = (\%\ OC)K_{ow} \tag{2.42}$$

where % OC the amount of organic carbon which is assumed 2% for soil and 4% for sediment and suspended solids.

From the investigation of Briggs [6], a regression equation between soil organic matter-water partition coefficient K_{om} and the n-octanol-water partition coefficient K_{ow} was established

$$\log K_{om} = (0.524 \pm 0.48)\log K_{ow} + (0.618 \pm 0.113) \qquad (2.43)$$

$$n = 30 \qquad r = 0.917$$

Karickhoff et al [41] correlated soil organic carbon-water partition coefficient, K_{oc}, and n-octanol-water partition coefficient, K_{ow}, for a series of polycyclic aromatics and chlorinated hydrocarbons ranging from 1 ppb to 1000 ppm in water solubility and obtained an excellent correlation

$$\log K_{oc} = -0.21 + 1.00 \log K_{ow} \qquad (2.44)$$

$$n = 10 \qquad r = 1.00$$

or

$$K_{oc} = 0.6\ K_{ow} \qquad (2.45)$$

$$n = 10 \qquad r = 0.96$$

Means et al [43] studied the relationship between soil organic carbon-water partition coefficient, K_{oc}, and n-octanol water partition coefficient, K_{ow}, for a variety of nonpolar compounds by various soils and sediments and they developed an equation describing this relationship

$$\log K_{oc} = \log K_{ow} - 0.317 \qquad (2.46)$$

$$n = 22 \qquad r = 0.98$$

Keenaga and Goring [6] correlated soil organic carbon-water partition coefficient, K_{oc}, and n-octanol-water partition coefficient K_{ow}, for several classes of compounds ranging from 0 to $1.2\text{x}10^6$ in K_{oc} and ranging from 10^{-4} to $3.7\text{x}10^6$ in K_{ow} and obtained two equations

$$\log K_{oc} = 1.377 + 0.544 \log K_{ow} \qquad (2.47)$$
$$n = 45 \qquad r = +0.86$$

$$\log K_{ow} = -1.070 + 1.358 \log K_{oc} \qquad (2.48)$$
$$n = 45 \qquad r = +0.86$$

Karichkhoff [42] correlated soil organic carbon-water partition coefficient, K_{oc}, and n-octanol-water partition coefficient, K_{ow}, for a group of polycyclic hydrocarbons including benzene, napthalene, phenanthrene, antracene and pyrene. The correlation equation was

$$\log K_{oc} = 0.989 \log K_{ow} - 0.346 \qquad (2.49)$$
$$n = 5 \qquad r = 0.997$$

Fitting the linear form gave

$$K_{oc} = 0.411\, K_{ow} \qquad (2.50)$$
$$n = 5 \qquad r = 0.994$$

In conclusion, reasonable estimation of the sorption behaviour of hydrophobic pollutants can be made from a knowledge of organic carbon contents of the soil or sediment and the n-octanol-water partition coefficient of the pollutant.

2.3.3 Correlation Between Soil Organic Carbon-Water Partition Coefficient, K_{oc}, and Water Solubility, S

The soil organic carbon-water partition coefficient, K_{oc}, represents the most useful and reproducible measure of comparative leachability in soil since the direct relationship of high water solubility to high leachability in soil and low water solubility to strong soil binding and reduced leaching has long been observed for many pesticides [6].

The sorption of ten hydrophobic aromatic and chlorinated hydrocarbons varying in water solubility from 1 ppb to 1000 ppm, on aquatic sediments was correlated with water solubility by Karickhoff et al [41]. The correlation between water solubility, S, and soil organic-water partition coefficient, K_{oc}, was given by an equation

$$\log K_{oc} = 0.44 - 0.54 \log S \qquad (2.51)$$

S = mole fraction, $n = 10$, $r = 1.00$

Keenaga and Goring [6] correlated water solubility and soil organic carbon-water partition coefficient, K_{oc}, for 106 compounds of several classes ranging in water solubility, S, from $1\text{x}10^{-4}$ ppm to $2.1\text{x}10^{6}$ ppm and ranging in soil organic carbon-water partition coefficient from 0 to $1.2\text{x}10^{6}$. Two regression equations were derived from this study

$$\log S = 5.09 - 1.28 \log K_{oc} \qquad (2.52)$$

S = ppm, $n = 106$, $r = -0.84$

$$\log K_{oc} = 3.64 - 0.55 \log S \qquad (2.53)$$

S = ppm, $n = 106$, $r = -0.84$

Means et al [43] studied the relationship between water solubility, S, and soil organic carbon-water partition coefficient, K_{oc}, for a group of compounds including pyrene, DMBA, 3 MC, and DBA on 14 soil and sediment samples exhibiting a wide range of physicochemical properties and obtain the following linear relationship

$$\log K_{oc} = -0.82 \log S + 4.070 \qquad (2.54)$$

$S = \mu g/l, \quad n = 4, \quad r = 1.000$

Karickhoff [42] studied correlation of soil organic carbon-water partition coefficient, K_{oc}, with water solubility, S, for polycyclic hydrocarbons including benzene, naphthalene, phenonthrene, anthracene and pyrene and obtained the following equation

$$\log K_{oc} = -0.594 \log S - 0.197 \qquad (2.55)$$

$S =$ mole fraction, $\quad n = 5, \quad r = 0.945$

When Karickhoff [42] examined the sorption behaviour of structural isomers, he saw that a crystal energy contribution in soil organic carbon-water partition coefficient, K_{oc}, estimation was necessary. Then, linear regression equation including crystal energy term was obtained. This crystal energy significantly improved the quality of fit to experimental data.

$$\log K_{oc} = -0.921 \log S - 0.00953(t_m - 25) - 1.405 \qquad (2.56)$$

$S =$ mole fraction, $\quad t_m = {}^\circ C, \quad n = 5, \quad r = 0.995$

For rigid organic molecules which are solids at 25°C, the crystal energy term is given by $-0.00953(t_m - 25)$ and for solutes that are liquids at 25°C, the melting point is set 25°C and the crystal energy term vanishes.

Karickhoff [42] suggested that Eq. (2.56) should work well for rigid hydrophobic organic solutes but for non-rigid molecules another crystal energy term was necessary. However, non-rigid molecules typically melted at much lower temperatures than rigid molecules of similar molecular weight and were frequently liquid at room temperature thus the crystal energy term was either zero or very small in most instances. The use of solubility with no crystal energy correction led to considerable error in K_{oc} estimation for organic solids containing polar functional groups (triazines and carbamates) and for anamalously high melting compounds. On the other hand, the corrected solubility equation apparently failed to extrapolate to high molecular weight chlorinated compounds (DDT, methoxychlor, hexachoro PCB's). It is suggested that overall for the vast majority of the available literature K_{oc} data, estimates derived from corrected solubilities were within the range of measurement variation, attributable to measurement error or reasonable differences in sediment soil sorption.

2.3.4 Correlation Between Bioconcentration Factor, K_B, and n-Octanol-Water Partition Coefficient, K_{ow}

A directly proportional relationship exists between bioconcentration factor and n-octanol-water partition coefficient.

Neely et al [35] established the first relationship between bioconcentration factor, K_B, and n-octanol-water partition coefficient, K_{ow}, in rainbow trout of a variety of chemicals over a wide range of partition coefficient in a flowing water ecosystem. An equation of the straight line of best fit was determined

$$\log K_B = 0.124 + 0.542 \log K_{ow} \qquad (2.57)$$

$$n = 8, \quad r = 0.948$$

Metcalf et al [46] showed the correlation between n-octanol-water partition coefficient, K_{ow}, and bioconcentration factor, K_B, with n-octanol-water partition coefficient from 1 to 4 for fish in the model ecosystem by the following equation [46]

$$\log K_B = 1.1587 \log K_{ow} - 0.7504 \qquad (2.58)$$

Lu and Metcalf correlated n-octanol-water partition coefficient, K_{ow}, with bioconcentration factor, K_B, in mosquito fish for eleven organic compounds using a static water ecosystem [6]. n-Octanol-water partition coefficient values was calculated from π values.

$$\log K_B = 0.7285 + 0.635 \log K_{ow} \qquad (2.59)$$

$$n = 11, \quad r = 0.7879$$

Lu et al in similar tests found that the log K_{ow} versus log K_B correlation of two carcinogens when plotted with the eleven compounds just mentioned fit the same regression equation [6].

Sugiura et al [46] studied on the bioconcentration of mono-, di-, and tetrachlorobiphyls and di-, tri-, and tetra-bromobiphenyls in the killifish. It was found that bioconcentration factors are proportional to n-octanol-water partition coefficients when the n-octanol-water partition coefficients are below 10^6, but not when the coefficients are above 10^6.

Veith et al compiled bioconcentration factor, K_B, and n-octanol-water partition coefficient, K_{ow}, data for 50 compounds and an equation derived from these data [38]

$$\log K_B = 0.85 \log K_{ow} - 0.70 \qquad (2.60)$$

$$n = 50, \quad r = 0.90$$

Keenaga and Goring [6] studied the relationship between n-octanol-water partition coefficient, K_{ow}, and bioconcentration factor, K_B, for a variety of compounds ranging from 0 to 6.16×10^4 in bioconcentration factor determined for flowing water systems and ranging from 1×10^{-4} to 3.6×10^6 in n-octanol-water partition coefficient. The relationship was given by two equations

$$\log K_{ow} = 2.312 + 0.809 \log K_B \qquad (2.61)$$

$$n = 26, \quad r = 0.87$$

$$\log K_B = -1.495 + 0.935 \log K_{ow} \qquad (2.62)$$

$$n = 26, \quad r = 0.87$$

Keenaga and Goring [6] also correlated n-octanol-water partition coefficient, K_{ow}, and bioconcentration factor, K_B, for 36 compounds varying in water solubility from 1×10^{-4} ppm to 2.1×10^6 ppm and varying in bioconcentration factor for static terrestrial-aquatic model ecosystem from 0 to 8.45×10^4 and two equations obtained from this correlation are

$$\log K_B = -0.973 + 0.767 \log K_{ow} \qquad (2.63)$$

$$n = 36, \quad r = 0.76$$

$$\log K_{ow} = 2.070 + 0.731 \log K_B \tag{2.64}$$

$$n = 36, \quad r = 0.76$$

Recently, Mackay [38] studied the relationship between bioconcentration factor, K_B, and n-octanol-water partition coefficient, K_{ow}, with the data set compiled by Veith, and by eliminating and exchanging some of them and adding new values from literature to the set, he obtained a new correlation.

$$\log K_B = \log K_{ow} - 1.32 \tag{2.65}$$

$$n = 59, \quad r = 0.95$$

or

$$K_B = 0.048 K_{ow} \tag{2.66}$$

If the actual bioconcentration factor is not known it can be predicted by using one of the correlation equations that has been established relating bioconcentration factor to either the n-octanol-water partition coefficient or to the water solubility of the chemical. Limitations to the use of these equations may occur with compounds that do not penetrate through tissues or bioconcentrate at the same rates in organisms as expected from the average molecule because of unusual steric configurations, molecular weights or solubilities [10]. A rapid metabolic alteration of a substance by organisms may result in its bioconcentration to a lesser extent than predicted [44].

2.3.5 Correlation Between Bioconcentration Factor, K_B, and Water Solubility, S

There is an inverse correlation between bioconcentration factor and water solubility.

Metcalf et al correlated water solubility, S, and bioconcentration factor, K_B, for twelve chlorinated hydrocarbons and DDT related insecticides using mosquitofish in his static terrestrial water ecosystem. When the results for hexachlorobenzene were excluded, a better correlation was obtained [6]

$$\log S = 5.99 - 1.176 \log K_B \tag{2.67}$$

S = ppb, $n = 12$, $r = -0.87$

Lu and Metcalf correlated water solubility, S, with bioconcentration factor, K_B, for mosquitofish obtained for eleven organic compounds under static exposure conditions [6] and obtained a correlation equation.

$$\log K_B = 3.9950 - 0.3891 \log S \tag{2.68}$$

S = ppb, $n = 11$, $r = -0.9228$

Chiou et al [17] correlated the water solubilities of seven organic chemicals with their bioconcentration factors from rainbow trout in flowing water tests. A regression equation was derived from this study

$$\log K_B = 3.41 - 0.508 \log S \tag{2.69}$$

S = µmol/l, $n = 7$, $r = -0.964$

Keenaga and Goring [6] studied the relationship between water solubility, S, and bioconcentration factor, K_B, for 36 compounds ranging in water solubility from 1×10^{-4} ppm to 2.1×10^{6} ppm and ranging in bioconcentration factor for flowing water tests from 0 to 6.16×10^{4} and two equations were obtained from this study

$$\log S = 2.531 - 0.916 \log K_B \tag{2.70}$$

S = ppm, $n = 36$, $r = -0.72$

$$\log K_B = 2.791 - 0.564 \log S \tag{2.71}$$

S = ppm, $n = 36$, $r = -0.72$

Keenaga and Goring [6] also correlated water solubility, S, and bioconcentration factor, K_B, for fifty compounds varying in water solubility from 1×10^{-4} ppm to 2.1×10^{6} ppm and varying in bioconcentration factor for static terrestrial aquatic model ecosystem from 0 to 8.45×10^{4} and two equations were obtained from this study

$$\log K_B = 2.183 - 0.629 \log S \tag{2.72}$$

S = ppm, $n = 50$, $r = -0.66$

$$\log S = 1.903 - 0.690 \log K_B \tag{2.73}$$

S = ppm, $n = 50$, $r = -0.66$

Recently, Mackay [38] obtained a relationship between bioconcentration factor and aqueous solubility

$$K_B = 86/S_L \tag{2.74}$$

where S_L is either the actual solubility in units of mole/m^3 if the solute is liquid or an estimated subcooled liquid solubility in units of mol/m^3 obtained from the actual solid solubility in units of mol/m^3 as

$$S_L = S_S \exp^{(-6.79(1-T_m/T))} \qquad (2.75)$$

in this equation S_L is the estimated subcooled liquid solubility in units of mol/m^3, S_S is the actual solid solubility in units of mol/m^3.

The correlations between bioconcentration factor and aqueous solubility allow an assessment of bioconcentration factor from aqueous solubility without requiring n-octanol-water partition coefficient.

2.3.6 Correlation Between Soil Organic Carbon-Water Partition Coefficient, K_{oc}, and Bioconcentration Factor, K_B

Keenaga and Goring [6] studied the relationship between soil organic carbon-water partition coefficient, K_{oc}, and bioconcentration factor, K_B, for 13 compounds varying from 0 to 1.2x10^4 in soil organic carbon-water partition coefficient and varying from 0 to 6.16x10^4 in bioconcentration factor for flowing water ecosystem and two equations were obtained from this study

$$\log K_{oc} = 1.963 + 0.681 \log K_B \qquad (2.76)$$

$$n = 13, \quad r = 0.87$$

$$\log K_B = -1.579 + 1.119 \log K_{oc} \qquad (2.77)$$

$$n = 13, \quad r = 0.87$$

Keenaga and Goring also correlated, K_{oc}, soil organic carbon-water partition coefficient and, K_B, bioconcentration factor for 22 compounds ranging from 0 to 1.2×10^6 in K_{oc} and ranging from 0 to 8.45×10^4 in K_B for static terrestrial aquatic ecosystem. Two equations were obtained from this study

$$\log K_{oc} = 1.886 + 0.681 \log K_B \qquad (2.78)$$
$$n = 22, \quad r = 0.91$$

$$\log K_B = -2.024 + 1.225 \log K_{oc} \qquad (2.79)$$
$$n = 22, \quad r = 0.91$$

2.3.7 Correlation Between Bioconcentration Factor for Flowing Water Ecosystem, $K_B(f)$, and Bioconcentration Factor for Static Terrestrial-Aquatic Ecosystem, $K_B(t)$

Keenaga and Goring [6] studied this correlation for 20 compounds ranging from 0 to 6.16×10^4 in bioconcentration factor for flowing water ecosystem and ranging from 0 to 8.45×10^4 in bioconcentration factor for static terrestrial-aquatic ecosystem and obtained two equations

$$\log K_B(t) = 0.717 + 0.703 \log K_B(f) \qquad (2.80)$$
$$n = 20, \quad r = 0.87$$

$$\log K_B(f) = 0.024 + 1.074 \log K_B(t) \qquad (2.81)$$
$$n = 20, \quad r = 0.87$$

III. MACKAY's LEVEL I FUGACITY MODEL

3.1 APPROACHES TO ENVIRONMENTAL EXPOSURE ANALYSIS

With the diversity of the chemicals that have been made, reasons for developing and improving the capability of estimating their behaviour in the environment are obvious. There have been numerous cases in which the health of humans and other organisms has been adversely affected by the indiscriminate emission or formation of chemicals that are biologically active. Some models have been developed which predict environmental behaviour of chemicals from their accessible physicochemical properties such as water solubility,S, vapor pressure,P,and n-octanol-water partition coefficient,K_{ow}. For the estimation of environmental exposure, the OECD Exposure Analysis Group initially considered four models [3].

(A) The Klöpffer Model which presumes equilibria between media

(B) The Neely Model [25,52] based on laboratory and monitoring data for a pesticide in a pond environment

(C) The Mackay Fugacity Model in which fugacity capacities are used to explain various compartment relationships [48-50].

This model can be used at several levels of sophistication depending on the available data.

(D) The Wood Model which is an adaptation of Mackay's Fugacity Model also has several levels.

The Klöpffer, Mackay, and Wood models make slightly different assumptions regarding compartment sizes but if no degradation processes are considered and the chemical's distribution across the environmental media is considered to be at equilibrium, they reduce to essentially the same set of equations.

It was decided not to consider two of the models in the context of OECD hazard assessment. The first was the Klöpffer model because it did not make provision for degradation or non-equilibrium processes, it was felt that the Neely Model applied to a specific experimental environment, and that it was difficult to defend its use as a general screening tool for a broad range of chemicals.

The two remaining models, the Wood and Mackay models, are both based on the concept of fugacity, i.e. the tendency for a substance to escape from a phase, and assume equilibrium or steady-state conditions among a set of environmental compartments. In their simpler versions (no degradation and instantaneous equilibration), these two models are identical in predicting environmental distribution. They both assume that

I. the environment is a closed system consisting of air (a), water (w), sediment (sd), soil (s), suspended solids (ss) and biota (b) compartments

II. the chemical has reached thermodynamic equilibrium in the environment both with respect to interphase transfer and intraphase transport

III. no degradation processes occur during the distribution.

3.2 FUGACITY AND FUGACITY CAPACITY CONCEPTS

If it is assumed that each compartment is well mixed, that is homogeneous and sufficient time has elapsed so that all compartments are in equilibrium then thermodynamics provides information about the nature of the partition. It is recognized that these assumptions are generally invalid because of in and outflows of a physical, chemical or biological nature but interestingly they tend to be most valid for persistant substances that are often of greatest toxicological concern.

Between phases equilibrium usually is achieved at considerably different concentrations. It is more illuminating to express these equilibrium partitioning situations in terms of fundamental quantity that controls the differing concentrations. Gibbs showed that diffusive equilibrium of a solute between two phases occurs when the chemical potentials of the solute in these phases are equal. Chemical potential is a difficult concept to grasp and use. Lewis introduced fugacity as a more convenient criterion for equilibrium between phases.

Fugacity is a thermodynamic quantity related to chemical potential or activity and characterizes the tendency for a substance to escape from a phase. It has units of pressure (whereas chemical potential has units of energy per mole, which is conceptually difficult to grasp). A chemical will diffuse from high to low fugacity. When equilibrium is achieved between two phases, the escaping tendencies from these phases are equal. (There may be transfer or exchange of solute between these two phases but the net rate of exchange is zero.)

A convenient property of fugacity is that it is usually linearly related to concentration at the low concentrations which are relevant to environmental contaminants. Just as temperatures (°C) can be related to heat concentrations (cal/m^3) using a proportionality constant heat capacity in units of cal/[m^3°C], fugacities can be related to concentrations using a similar fugacity capacity constant, Z with units of mol/[m^3Pa]

$$C = f.Z \tag{3.1}$$

where C is concentration in units of mol/m^3, f is fugacity in units of Pa and Z is "fugacity capacity" in units of mol/[m^3Pa].

The fugacity capacity Z, which quantifies the capacity of the phase for fugacity, depends on temperature, pressure, the nature of the substance and the medium in which it is present.

The magnitude of Z values gives a direct indication of the likely concentration. At a given fugacity if Z is low, C is low; if Z is high, C is high. Thus high concentrations can be reached without creating high fugacities. For example, the fugacity capacity Z for oxygen in water at room temperature is 1.5 gmol/m^3atm, in air it is 40 gmol/m^3atm, a ratio of about 27. Oxygen then adopts a concentration in air 27 times that in water (a concentration of 0.3 mol/m^3 in the water and 8.0 mol/m^3 in the air).

Mass tends to accumulate in phases where fugacity capacity is largest. Apparently, hydrophobic organics tend to partition into lipid phases because that is where their Z value is largest.

If there are two phases, then equilibrium of a substance will be reached when the fugacities are equal, that is

$$f_1 = f_2 \tag{3.2}$$

thus

$$C_1/Z_1 = C_2/Z_2 \tag{3.3}$$

or

$$C_1/C_2 = Z_1/Z_2 = K_{12} \tag{3.4}$$

The concentration ratio which is the partition coefficient controlling the distribution of the substance between two phases is simply the ratio of the fugacity capacities.

Expressing equilibrium in terms of fugacity capacities is more convenient because it separates the escaping tendencies of the chemical from each phase and facilitates the calculation of these quantities from other related thermodynamic data.

If we can find Z for a substance for each environmental phase we can easily calculate how the substance will partition.

3.3 FUGACITY CAPACITY CALCULATIONS

Z values for a substance for each environmental phase can be calculated from physical-chemical data and partition coefficients as given by Mackay [49]

3.3.1 Fugacity Capacity for the Atmosphere, Z_a

In the vapor phase, the fugacity is rigorously expressed by

$$f = y\phi P_T \simeq P \tag{3.5}$$

where y is the substance's (solute's) mole fraction, P_T is the total pressure (here atmospheric pressure) in unit of Pa, ϕ is the fugacity coefficient which is dimensionless and is introduced to account for nonideal behaviour. Fortunately, at atmospheric pressure, ϕ is usually close to unity and can thus be ignored. The exceptions are solutes such as carboxylic acids, that associate in the vapor phase.

The fugacity is thus equivalent, in most cases, to the partial pressure, P. It should be noted that this equation assumes the solute to be in truly gaseous form, not associated with particles. Concentration C is related to partial pressure through the gas law

$$C = n/V = P/RT = f/RT = fZ \tag{3.6}$$

Thus Z_a for vapors is simply 1/RT and has a value of 4.04×10^{-4} mol/(m Pa) corresponding to R of 8.31 (pa.m^3)/(mol.°K) or J/(mol °K), and a temperature of 25°C (298°K). Z_a is independent of the nature of the solute or the composition of the vapor (for nonassociating solutes and low - or atmospheric- pressure conditions) and has an obvious temperature dependence.

3.3.2 Fugacity Capacity for Water, Z_w

In aqueous solution, the fugacity is given by

$$f = x\gamma P^S \tag{3.7}$$

where x is the mole fraction; P^S is the vapor pressure of the pure liquid solute at the system temperature; and γ is the liquid-phase activity coefficient on a Raoult's Law convention. By this convention, when x is unity, γ is also unity, and f becomes the pure liquid state component vapor pressure. Generally, for nonionizing substances, γ increases to an "infinite dilution" value as x tends to zero. This relationship between x and γ is often of the form

$$\ln \gamma = K(1 - x)^2 \tag{3.8}$$

In most environmental situations, x is quite small; thus, ln γ can be equated to K without serious error. This near constancy in γ leads to the very convenient near-linear relationship between C and f, reflected as a constant value in Z.

The relationship between f and C to give Z for infinite dilution conditions can be obtained by writing

$$Z_W = C/f = C/P = 1/H = x/v_W f = 1/v_W \gamma P^S \tag{3.9}$$

where v_W is the molar volume (m^3/mol) of the solution, which is approximately that of water (1.8×10^{-5} m^3/mol).

For water, Z_W is simply the reciprocal of Henry's Law constant.

3.3.3 Fugacity Capacity for Sorbed Phases (soil, sediment or suspended solids) Z_S, Z_{sd}, Z_{ss}

Sorption equilibria are usually expressed as equations or isotherms relating dissolved to sorbed concentrations. Examples are the Freundlich, BET, Langmuir or linear equations for most hydrophobic compounds at concentrations well below their solubilities linear equation is adequate

$$x = K_pC \tag{3.10}$$

where x is the sorbed concentration expressed as mol solute/10^6g sorbent (wet or dry) and K_p is a sorption coefficient with units of m^3 water/10^6g sorbent. The equation is often expressed in mass concentration units x in g/10^6g or µg/g and C in g/m^3 or mg/liter in which case an identical numerical value is obtained for K_p.

If the sorbent concentration expressed as volume fraction is *s* and its density is ρ g/cm^3 or 10^6g/m^3, then its concentration is *s* 10^6g/m^3 or g/cm^3. The concentration of sorbed material C_s, expressed as mol/m^3 sorbent, is thus xρ mol/m^3.

At equilibrium, the fugacities of the sorbed and dissolved material must be equal, so if Z_s is the sorbed phase fugacity capacity

$$f = HC = C_s/Z_s \tag{3.11}$$

then

$$Z_s = C_s/HC = x\rho/H(x/K_p) \tag{3.12}$$

and

$$Z_s = K_p\rho/H \tag{3.13}$$

The group $K_p\rho$ is dimensionless.

3.3.4 Fugacity Capacity for Biotic Phases, Z_b

For biota, a bioconcentration factor K_B is used instead of the partition coefficient. If it is expressed as a ratio of the concentrations in the biota (say fish) on a wet weight basis and in the water, it is identical to K_p. If expressed on a wet volume basis, it is rigorously analogous to the group K_p where is the fish density.

$$Z_b = K_B\rho/H \qquad (3.14)$$

3.3.5 Fugacity Capacity for Pure Solid and Liquid Phases, Z_p

For pure solid or liquid substances, the fugacity is the vapor pressure. The substance's concentration of C is the inverse of the molar volume, v_s in units of m^3/mol. Thus Z_p is given by

$$Z_p = C/f = 1/P^S v_s \qquad (3.15)$$

Such phases occur environmentally only when the solute solubility in a phase is exceeded and "precipitation" occurs.

3.3.6 Fugacity Capacity for Inert Solutes

Some substances, such as ceramic or mineral matter, polymers, metals, and sparingly soluble metal salts do not partition appreciably between environmental media and their appropriate Z values are unavailable. The thermodynamic explanation is that such substances have near-infinite Z values in their pure solute form because of very low values of P^S.

3.4 ENVIRONMENTAL APPLICATIONS OF THE FUGACITY-CONCENTRATION APPROACH

There are two general areas in which the fugacity concentration approach can contribute to a better understanding of the fate of toxic substances

$$C = f.Z \tag{3.1}$$

First, if concentration data are available for a pollutant in several phases, presumably as a result of monitoring program, these concentration data can be converted to fugacities and the fugacity levels compared. Examination of fugacity levels in various environmental compartments thus provides an insight into sources, transportation routes, and directions, and to regions in which transformation or other removal processes occur.

The second application is the prediction of the likely environmental distribution of a compound between environmental compartments. To apply this approach a model environment must be designed. The volumes and properties of compartments must be selected to mimic as closely as possible a real environment.

3.5 SELECTION OF MODEL VOLUMES

In order to calculate environmental partitioning in the form of amounts in each medium, it is necessary to assume volumes for each medium and an amount of solute. Clearly, any concentration can be obtained by the selection of suitable volumes and solute amount, thus only the relative concentrations have significance. The mass distribution depends on the assumed phase volumes; therefore the results are reasonable only to the extent that the volumes are reasonable. Further, selection of suspended matter concentrations, biota concentrations and organic carbon contents of soils and sediments affect the results.

The "unit world" designed by Mackay and Neely [51] are considered reasonable for evaluation purposes. This unit world as illustrated in Figure 3.5.1 consists of 1 km square with a 6 km high atmosphere; 30% of the area is covered by soil having a depth of 15 cm and 70% is water covering an average depth of 10 m, with 3 cm of sediment, 5 ppm by volume of suspended solids and 1 ppm of biota. The densities are 1000 kg/m^3 for water and biota, 1500 kg/m^3 for solid phases and 1.19 kg/m^3 for air [49-51]. The organic carbon contents are 2% for soil and 4% for sediment and suspended solids. A temperature of 25°C is assumed.

The total amounts of solute are chosen to be 100 mol.

The soil water partition coefficient is calculated from n-octanol-water partition coefficient by using Karickhoff's correlation which has a high correlation coefficient (r = 1.00)

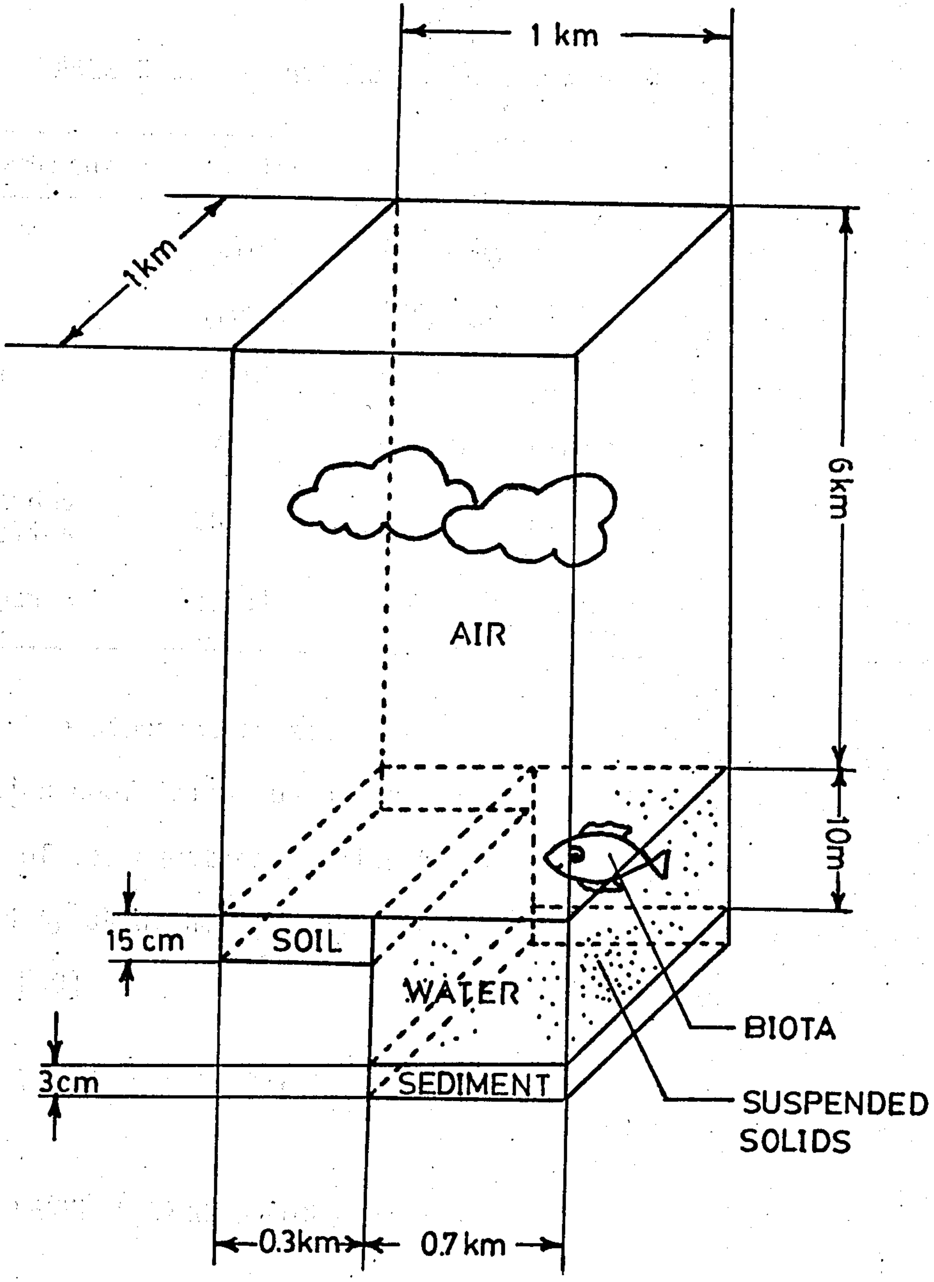
$$K_p = (\%\ OC)K_{oc} \qquad (2.42)$$

and

$$\log K_{oc} = -0.21 + 1.00 \log K_{ow} \qquad (2.44)$$

or

$$K_{oc} = 0.6\ K_{ow} \qquad (2.45)$$



GURE 3.5.1 Unit world designed by Mackay and Neely [50]

thus

$$K_p = \% \, OC(0.6 \, K_{ow}) \tag{3.15}$$

TABLE 3.5.1 - Unit World Compartment Volumes and Densities [50,51]

Compartment	Volume (m³)		Density (kg/m³)
Air	$6x10^9$	(1 kg²area x 6 km height)	1.19
Soil	$4.5x10^4$	(30% area x 15 cm depth)	1500
Water	$7x10^6$	(70% area x 10 m depth)	1000
Biota	7	(Water volume x 1 ppm)	1000
Suspended Solids	35	(Water volume x 5 ppm)	1500
Sediment	$2.1x10^4$	(70% area x 3 cm depth)	1500

The bioconcentration factor is calculated from n-octanol-water partition coefficient by using Veith's correlation, since this equation is one of the equations having the highest correlation coefficient derived by using high number of compounds and also it is used by Mackay [49]

$$\log K_B = 0.85 \log K_{ow} - 0.7 \tag{2.60}$$

3.6 LEVEL I CALCULATIONS

In level I calculations, the equilibrium distribution of a fixed amount of non-reacting compound (arbitrarily chosen to be 100 moles) in the evaluative environment is calculated using fugacity capacities that are calculated from physical-chemical data and partition coefficients.

The equilibrium ratios of concentrations and the relative amounts in each phase are obtained. This first step calculations answer the questions where will the chemical go in the environment and what will be its relative concentrations.

These level I calculations give no information about reactivity or persistence. More complex fugacity models are used to compare additional features.

In level I calculations, it is assumed that

(A) the environment is a closed system consisting of air (a), water (w), sediment (sd), soil (s), suspended solids (ss), and biota (b) compartments

(B) the chemical has reached thermodynamic equilibrium in the environment both with respect to interphase transfer and intraphase transport

(C) no degradation process occur during the distribution.

Under these conditions, the escaping tendencies from all phases are equal so that a common fugacity (f) prevails

$$f_a = f_s = f_w = f_b = f_{ss} = f_{sd} = f \qquad (3.16)$$

If each phase in equilibrium has a volume of V_i (m^3) and fugacity capacity, Z_i, then the concentration in each phase, C_i (mole/m^3)

$$C_i = f\,Z_i \qquad (3.17)$$

where f is the prevailing common fugacity.

The amount of material in each phase, M_i (mole) thus

$$M_i = C_iV_i = f\ Z_iV_i \tag{3.18}$$

and the total amount M_T (mole)

$$M_T = f\ \Sigma Z_iV_i \tag{3.19}$$

Since the total amount is known, the fugacity can thus be calculated as

$$f = M_T/\Sigma\ Z_iV_i \tag{3.20}$$

Hence, the individual values of C_i and M_i can be deduced.

$$C_i = f\ Z_i \tag{3.21}$$

and

$$M_i = C_iV_i \tag{3.22}$$

Mass partitioning among the compartments can be calculated according to

$$P_i = Z_iV_i/\Sigma_i\ Z_iV_i \tag{3.23}$$

And equilibrium partitioning fractions can be calculated as

$$P_i' = Z_i/\Sigma_i\ Z_i \tag{3.24}$$

It is clear that these calculations give two different classes of information - where the most of the solute partitions and where the highest concentration occur.

3.7 ENVIRONMENTAL EXPOSURE ANALYSIS

This simple fugacity model is quite hypothetical since it ignores inputs outputs and transformations and it assumes that intercompartment transfer is fast. The behaviour and concentratons in the real environment will differ from those calculated but the dominant behaviour characteristics should be mimicked. The value of the model lies in identifying compartments in which the bulk of a contaminant will tend to accumulate and in which its residues should sought or in which degradative processes are likely to be important. It merely represents a picture of ultimate distribution of the substance in the environment in terms of both relative concentrations and relative masses and thus providing comparative exposure information about chemicals, assists priority setting.

The results obtained for each chemical can be designed to yield relative rank of importance for each compartment. The advantage of this ranking is that it makes the chemicals with the greatest potential to contaminate for a compartment quite obvious. The next step would be to examine these chemicals critically to see if they truly are a problem. If the degradation of a chemical exists in a compartment its actual concentration in that compartment will be lesser than its expected maximum potential concentration.

3.8 CRITERIA

It is generally accepted that models should be validated by comparison with real environmental data. Models of the type described here are "evaluative" and do not purport to describe any particular real environment, or do not purport to calculate the actual solute concentrations or their precise behaviour in the environment thus they cannot be validated except by general comparison of observed environmental concentrations with the predicted values. Since the models are based on valid physical laws, the behaviour expressed should be in broad agreement with environmental behaviour.

The level I Fugacity Model's applicability was first examined by hindcasting the distribution of 2,4,5,4',5'-pentachlorobiphenyl by Mackay et al [51]. It is known that the predicted compartment concentrations are controlled by two factors other than their physicochemical properties these are the amounts introduced (arbitrarily chosen to be 100 moles) and the compartment volumes which are based on reasonable literature values [51]. It is found that the model predicts a concentration which is within an order of magnitude of those found in practice' thus water concentrations are predicted to be in the parts per trillion range and sediment and biota concentrations to be sub-parts-per-million-range - both of which predictions are realistic. The largest discrepancy is in the predicted atmospheric concentrations which are about three orders of magnitude higher than those found. The discrepancy arises because this version of the model predicts equilibrium distributions based on thermodynamic criteria without taking into account the kinetics of air-water exchange processes which limit atmospheric concentrations as suggested by Mackay et al. Level I fugacity model predicts reasonable concentrations and ratios of concentrations in compartments other than atmosphere.

IV. USE OF MODEL OUTPUTS FOR HAZARD ASSESSMENT

4.1 A DECISION TREE

It is generally accepted that before a new chemical compound is released into the market and thus into the environment, it should undergo some assessment of its likely environmental impacts. Knowing how a chemical behaves in the environment is particularly important in determining whether a chemical will come in contact with a critical species or man and perhaps cause a toxic effect or, in contrast, be rapidly degraded to innicouous materials. A decision tree was designed for an appropriate environmental testing program by Neely [2] as represented in Figure 4.1.1. The lettered boxes in Figure 4.1.1 will be described below. The YES output from Boxes K, L, and M indicate the need for further studies on degradation. Main degradation processes in the environmental compartments are given in Table 4.1.1.

(A) Use Pattern

A brief description of the product should be given indicating how the material will be used. In addition to the use pattern an

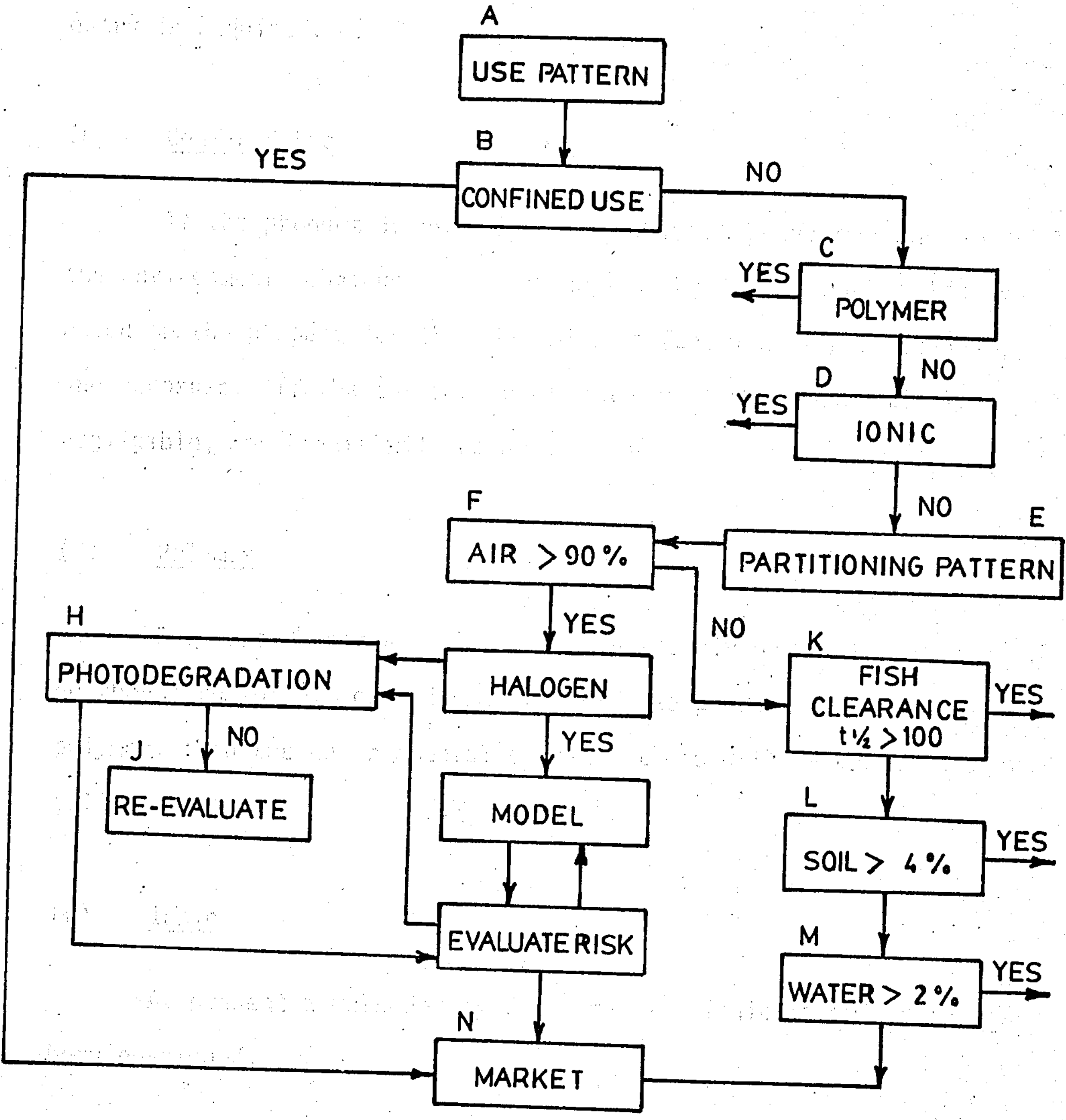


FIGURE 4.1.1. Schematic representation of a decision tree for designing an appropriate environmental testing [2]

estimate of the initial amount and planned rate of environmental entry is required.

(B) Confined Use

If the product is used in a manner which prevents entry into the environment, obviously no further testing is required. This is based on the proposition that hazard is a function of both toxicity and exposure. If the environmental concentration is essentially negligible, the hazard will be negligible.

(C) Polymer

Polymers do not normally exist in the air or water phases nor do they sorb to soil organic matter. If the product is an insoluble polymer, then the environmental considerations will be associated with solid waste.

(D) Ionic

At present a methodology for screening ionic materials has not been developed.

(E) Partitioning Pattern

By using the chemical and physical properties of a chemical through a model the partitioning of that chemical between environmental compartments can be quickly assessed.

TABLE 4.1.1 - Main Degradation Processes by Environmental Compartments

AIR (TROPOSPHERE)

- Photolysis
- Oxidation (HO· and O_3)

SURFACE WATER and TOPSOIL

- Hydrolysis
- Biodegradation by aerobic bacteria
- Photolysis
- Oxidation ($RO_2\cdot$)

SEDIMENT

- Hydrolysis
- Biodegradation by anaerobic bacteria

(F) Air > 90%

If the results of the analysis in E indicate that 90% or greater of the chemical is in the air compartment proceed to G, otherwise proceed to K.

(G) Halogen

If the agent contains halogen, an analysis of the mass entering the stratasphere should be conducted. This is based on the theory that chlorine and bromine atoms will cause an increase in the rate at which stratosphere ozone is destroyed. Models have been proposed to estimate the transfer of chlorine from the troposphere to the stratosphere. Any suitable model can be used as long as the same technique is used for all cases. Based on the results of the analysis, decisions can be made about the relative risk. It may be desirable to obtain further data as indicated in Figure 4.1.1, with the arrow entering box H from the "Evaluate Risk" box and the information generated recycled back through the model. If the volatile chemical does not contain halogen proceed to box H.

(H) Photodegradation Potential

Those chemicals containing C-H or C=C bonds will be susceptible to hydroxyl radical attack in the troposphere and will be degraded. In such a situation no tropospheric build up will occur. If the use pattern indicates that no potential problem is perceived in a local environment go to N.

(J) Reevaluate

Once a material enters this box on the first pass, a reevaluation of the properties is necessary. If continued development is warranted, then obviously a search for other degradation pathways must be conducted.

(K) Fish Clearance

Fish clearance half life time, $t_{1/2}$ is the interval of time needed for a 50% decrease of a given concentration of a chemical present in an organism after termination of exposure [45]. It can be easily calculated from physical chemical properties of chemical by using the equation given by Neely [2]

$$\log t_{1/2} = 0.0027(1/H) - 0.282 \log (S/M) + 1.08 \qquad (4.1)$$

where $t_{1/2}$ is the half life for clearance from fish in unit of hours, H is the Henry's Law constant in units of mm Hg $m^3 mole^{-1}$, S is the water solubility in units of ppm, M is the molecular weight of chemical in unit of gram.

If $t_{1/2}$ is greater than 100 hours, a potential problem of bioconcentration is indicated. If the chemical screened has this high a number, it should be examined experimentally for degradability and possibly bioconcentration in aqueous systems. If $t_{1/2}$ is less than 100 hours proceed to L.

(L) Soil > 4%

If the amount of a chemical in the soil compartment is greater than 4%, degradation in soil needs to be investigated.

(M) Water > 2%

If the amount of chemical in the water compartment is greater than 2%, degradation studies are required.

(N) Manufacturing Decision

Based on the use pattern, no long-term environmental problem is anticipated and production of the chemical should proceed. Testing should be continued until enough is known about degradation, distribution and toxicity of the compound to insure that the expected environmental concentration resulting from the use is below the no-effect level. Once this is demonstrated manufacture and distribution should be allowed.

The proposed decision tree does have the capability of quickly focusing on the key areas for further testing. It also serves as an alert system for what precautions are necessary in both the manufacturing and distribution of the product.

4.2 IMPORTANCE (OR ADVANTAGE) OF PRELIMINARY ASSESSMENTS

The total universe of chemicals which was given by the EPA Toxic Substance Inventory List consists of 40,000 entries in annual production of 1.8×10^{12}kg (4×10^{12}pounds) [1]. With the diversity of the chemicals that have been made, there is a need for a program to assess the potential environmental hazard resulting from the use of various products. Without such a program, the task of experimentally making an assessment for each chemical becomes impossible. It will be impossible for the reason that the man power and resources available are not equal to the task. Furthermore the need for performing all conceivable tests is not necessary. The decision tree will be helpful in order to ensure that critical tests are performed and to prevent needless experimentation.

The objective of this approach is to enable the studies to proceed in a logical manner and to optimize the amount of information in a cost effective manner, because analysis of the resulting pattern indicates the compartment offering the best chance for maximum degradation, and then further environmental tests if needed can be designed in a logical and sequential manner. By being aware of the potential environmental problems before they occur, greater precautionary measures can be taken in both the manufacture and distribution of the material.

V. THE PREDICTED ENVIRONMENTAL DISTRIBUTION OF SUBSTITUTED BENZENE DERIVATIVES

For benzene and 72 substituted benzenes, the potential concentrations and equilibrium distributions between the compartments of an evaluative environment are calculated by using Mackay's Level I fugacity model and their ranking by their potentials to contaminate each compartment is given.

5.1 INPUT DATA

The fundamental physical chemical properties of benzene and 72 substituted benzene derivatives such as water solubility, vapor pressure, n-octanol-water partition coefficient are compiled in Table A.2.1.

5.1.1 Water Solubility

Water solubility data in units of g/m^3 obtained from several papers and handbooks [1,2,6,7,8,11-27] are compiled in Table A.2.1. Only six of them are calculated from n-octanol-water partition coefficients which are also given in Table A.2.1 by using Chiou's correlation equation (2.33). This equation is used since the chemicals, solubilities of which calculated here are liquids or low melting solids and that equation being one of the equations which have the highest correlation coefficients derived from high number of compounds is suitable for their calculations and these calculated values are designated by "calc 1" in Table A.2.1.

$$\log K_{ow} = 5.00 - 0.670 \log S \qquad (2.33)$$

where S = water solubility in mol/liter, K_{ow} = n-octanol-water partition coefficient.

Specimen Calculation

As given in Table A.2.1, m-ethyl phenol has a log K_{ow} of 2.4 and molecular weight of 122.17 gr. Then its water solubility can be quickly calculated by using Chiou's correlation Eq. (2.33)

$$\log K_{ow} = 5.00 - 0.670 \log S$$

$$2.4 = 5.00 - 0.670 \log S$$

$$S = 7596.2\ \mu\text{mol/liter}$$

$$S = 7596.2\ \mu\text{mol/liter} \times 122.17\ \mu\text{gr}/\mu\text{mole} \times 10^{-6}\ \text{gr}/1\ \mu\text{gr} \times 10^{3}\text{liter}/1\ \text{m}^3$$

$$S = 928.03\ \text{g/m}^3.$$

5.1.2 Vapor Pressure

In addition to some vapor pressure values taken from literature [22,1,13,25,7,28], many calculated vapor pressure values in units of mm Hg are compiled in Table A.2.1.

Some of them are calculated by using the Antoine Equation (Eq. 2.12)

$$\log P = A - B/(t + C) \tag{2.12}$$

where P = vapor pressure in mm Hg, A, B and C are Antoine constants, t = system temperature in °C.

While the values calculated by using Antoine constants taken from Ref. 30 are designated by "calc 2", those that are calculated by using Antoine constants taken from list of Boublik et al [31] are designated by "calc 4" in Table A.2.1.

Antoine constants used for calculations listed in Table A.2.2 with references from which they are taken.

Specimen Calculation

As given in Table A.2.1, Benzene has 2 sets of Antoine constants taken from two different references [30-31]. $A = 6.9057$, $B = 1211.03$, $C = 220.79$ from Ref. 30 and $A = 6.8927$, $B = 1203.53$, $C = 219.88$ from Ref. 31. By using Antoine Equation (2.12), for 25°C two pressure values are obtained according to available constants.

$$\log P = A - B/(C + t) \tag{2.12}$$

$$\log P = 6.9057 - 1211.03/(220.79 + 25)$$

$$\log P = 1.9786$$

$$P = 95.194 \text{ mm Hg}$$

and

$$\log P = 6.8927 - 1203.53/(219.88 + 25)$$

$$\log P = 1.9779$$

$$P = 95.044 \text{ mm Hg}$$

In Table A.2.1, first one is designated by "calc 2", and the second one is designated by "calc 4".

The values designated as "calc 3" in that table are calculated by using Antoine Equation in the form of Eq. 2.13 when only two constants B and C are available in Table A.2.2.

$$\log P = (-52.23B/T) + C \qquad (2.13)$$

where P = vapor pressure in mm Hg, B and C = Antoine constants, T = system temperature in °K.

Specimen Calculation

As given in Table A.2.2, Acetophenone has only two constants B and C for a temperature range of 30°C to 100°C, B = 55.170, C = 9.1352.

For T = 298.16°K

$$\log P = (-52.23B/T) + C$$

$$\log P = ((-52.23 \times 55.117)/298.16) + 9.1352$$

$\log P = -0.5199$

$P = 0.3021$ mm Hg.

Most of the halobenzenes have no available vapor pressure data in literature other than boiling and melting points listed in Table A.2.3. In that case, vapor pressures are obtained by using Kistiakowsky Linear ΔH (KLH) equation which can be applied only to hydrocarbons and halogenated hydrocanbons (Eq. (2.14))

$$\ln P = -(4.4 + \ln T_B)\{1.803((T_B/T) - 1) - 0.803 \ln(T_B/T)\} - 6.8((T_M/T) - 1)$$

where P = vapor pressure in atm at environmental temperature T in °K T_B and T_M = boiling and melting point temperatures in °K. The third term including melting point is ignored for liquids.

In Table 5.1.1, the vapor pressure values calculated by using KLH equation are designated by "calc 5". For these calculations the boiling and melting point temperatures are taken from Table A.2.3.

Specimen Calculation

As given in Table A.2.3, o-difluorobenzene is a liquid having a melting point of -34°C and a boiling point of 92°C. On the other hand, p-dibromo benzene is a solid having a melting point of 87°C and a boiling point of 219°C.

For o-difluorobenzene (liquid)

$T_M = -34 + 273.16 = 239.16$°K

$T_B = 92 + 273.16 = 365.16$°K

$T = 298$°K

$$\ln P = -(4.4 + \ln T_B)\{1.803((T_B/T) - 1) - 0.803 \ln(T_B/T)\}$$

$$\ln P = -(4.4 + \ln 365.16)\{1.803((365.16/298.16) - 1) - 0.803 \ln(365.16/298.16)\}$$

$$\ln P = -2.4966$$

$$P = 0.0824 \text{ atm}$$

$$P = 0.0824 \times 760 = 62.596 \text{ mm Hg.}$$

For p-dibromobenzene

$T_M = 87 + 273.16 = 360.16°K$

$T_B = 219 + 273.16 = 492.16°K$

$T = 298.16°K$

$$\ln P = -(4.4 + \ln T_B)\{1.803((T_B/T) - 1) - 0.803 \ln(T_B/T)\} - 6.8((T_M/T) - 1)$$

$$\ln P = -(4.4 + \ln 492.16)\{1.803((492.16/298.16) - 1) - 0.803 \ln(492.16/298.16)\} - 6.8((360.16/298.16) - 1)$$

$$\ln P = -9.581$$

$$P = 6.9 \times 10^{-5} \text{ atm}$$

$$P = 6.9 \times 10^{-5} \times 760 = 0.05246 \text{ mm Hg.}$$

Some of the vapor pressures in Table A.2.1 are calculated by using Eq. (2.11) to obtain a value of log P_2 for a temperature T_2 from values of log P_1 and log P_3 for temperatures T_1 and T_3. The vapor pressure temperature data [34] used for calculation are given in Table A.2.4. These calculated values are designated by "calc 6" in Table A.2.1.

$$\log P_2 = \log P_1 + (\log P_3 - P_1)(T_2 - T_1)T_3/(T_3 - T_1)T_2 \quad (2.11)$$

where P = vapor pressure in mm Hg, T = absolute temperature in °K.

Specimen Calculations

(A) As given in Table A.2.4, fluorobenzene has vapor pressure values of P_1 = 60 mm Hg at 19.6°C and P_3 = 100 mm Hg at 30.4°C and P_2 at 25°C.

$T_1 = 19.6 + 273.16 = 292.76°K$

$P_1 = 60$ mm Hg

$T_2 = 25 + 273.16 = 298.16°K$

$T_3 = 30.4 + 273.16 = 303.56°K$

$P_3 = 100$ mm Hg

and then

$$\log P_2 = \log P_1 + (\log P_3 - \log P_1)(T_2 - T_1)T_3/(T_3 - T_1)T_2$$

$$\log P_2 = \log 60 + (\log 100 - \log 60)(298.16 - 292.76)303.56/(303.56 - 292.76)298.16$$

$$\log P_2 = 1.8911$$

$$P_2 = 77.819 \text{ mm Hg}$$

(B) As given in Table A.2.4, bromobenzene has vapor pressure values of P_2 = 5 mm Hg at 27.8°C and P_3 = 10 mm Hg at 40°C and P_1 mm Hg at 25°C

$T_1 = 25 + 273.16 = 298.16$ °K

$T_2 = 27.8 + 273.16 = 300.96°K$

$P_2 = 5$ mm Hg

$T_3 = 40 + 273.16 = 313.16$°K

$P_3 = 10$ mm Hg

and then

$$\log P_2 = \log P_1 + (\log P_3 - \log P_1)(T_2 - T_1)T_3/(T_3 - T_1)T_2$$

$$\log 5 = \log P_1 + (\log 10 - \log P_1)(300.96 - 298.16)313.16/(313.16 - 298.16)300.96$$

$$0.69897 = \log P_1 + (1 - \log P_1)0.19423$$

$$\log P_1 = 0.6264$$

$$P_1 = 4.23069 \text{ mm Hg}$$

5.1.3 n-Octanol-Water Partition Coefficient

In addition to values taken from literature [6,7,11,16-20,22,23,26,35,37,38], most of the n-octanol-water partition coefficients in Table A.2.1 are calculated from substituent constant, π, values by using Eq. (2.21)

$$\log K_{ow}(RX) - \log K_{ow}(RH) = \pi(X) \qquad (2.21)$$

where $\log K_{ow}(RX)$ = the logarithm of the partition coefficient of the chemical in question, $\log K_{ow}(RH)$ = the logarithm of the partition coefficient of the parent structure, π = substituent constant representing the contribution of each group to the parent structure that give $K_{ow}(RX)$.

The π values listed in Table A.2.5 was determined by Fujita et al [36] experimentally. The following values for log K_{ow} enables one to calculate K_{ow} for any of the compounds listed in Table A.2.5. For phenol log K_{ow} = 1.46 ± 0.01, for aniline log K_{ow} = 0.90 ± 0.01, for nitrobenzene log K_{ow} = 1.85 ± 0.01, for benzene log K_{ow} = 2.13 ± 0.01

Specimen Calculation

As given in Table A.2.5, the substituent constant for fluorine on benzene is 0.14 ± 0.02 and benzene has a log K_{ow} of 2.13 ∓ 0.01 then by using Eq. (2.21) the log K_{ow} of fluorobenzene can be quickly calculated.

$$\log K_{ow}(RX) = \log K_{ow}(RH) + \pi(X)$$
$$\log K_{ow}(C_6H_5\text{-}F) = \log K_{ow}(C_6H_6) + \pi(F)$$
$$\log K_{ow}(C_6H_5\text{-}F) = 2.13 \pm 0.01 + 0.14 \pm 0.02$$
$$\log K_{ow}(C_6H_5\text{-}F) = 2.27 \pm 0.03$$

In Table A.2.1 n-octanol-water partition coefficient values calculated from π substituent constants given in Table A.2.5 by using Eq. (2.21) are designed as "calc 7".

Only a few of the n-octanol-water partition coefficients in Table A.2.1 are calculated from f, hydrophobic fragmental constants listed in Table A.2.6 by using Eq. (2.23) and these calculated values are designated by "calc 8"

$$\log K_{ow}(RX) = f(R) + f\ (X) \qquad (2.23)$$

where f = the hydrophobic fragmental constant being lipophilicity contribution of a constituent part of a structure to the total lipophilicity, low $K_{ow}(RX)$ = the logarithm of partition coefficient of the chemical in question.

Specimen Calculation

As given in Table A.2.6, the hydrophobic fragmental constant for fragment I is 1.460, for fragment C_6H_5 1.90. Then the log K_{ow} value of Iodobenzene can be quickly calculated by using Eq. (2.23).

$$\log K_{ow}(C_6H_5.I) = f(C_6H_5) + f(I)$$

$$\log K_{ow}(C_6H_5.I) = 1.90 + 1.460$$

$$\log K_{ow}(C_6H_5.I) = 3.36$$

Only two of the n-octanol-water partition coefficients in Table A.2.1 are calculated from solubility by using Chiou's equation (Eq. 2.33). These calculated values are designated by "calc 9".

$$\log K_{ow} = 5.00 - 0.670 \log(S \times 10^3/M) \qquad (2.33)$$

where K_{ow} = n-octanol-water partition coefficient, S = water solubility in ppm, M = molecular weight in gr.

Specimen Calculation

m-Phenylene diamine has a value of solubility 25×10^4 g/m^3 and a value of molecular weight 108.15 gr then by using Chiou's correlation, n-octanol-water partition coefficient is easily calculated.

$$\log K_{ow} = 5.00 - 0.670 \log(S \times 10^3/M)$$

$$\log K_{ow} = 5.00 - 0.670 \log(25 \times 10^4 \times 10^3/108.15)$$

$$\log K_{ow} = 0.7362$$

$$K_{ow} = 5.44725$$

Input data given in Table A.2.7 and used for calculations are obtained from the values given in Table A.2.1.

5.2 CALCULATIONS

In this study, for benzene and 72 substituted benzenes, the potential concentrations and equilibrium distributions between the environmental compartments are calculated by using Mackay's Level I Fugacity Model given in Chapter III and Input data given in Table A.2.7. The calculations are performed on a CDC Cyber 170 Computer.

5.2.1 The Computer Program Used for Calculations

Two computer programs based on Mackay's Level I fugacity model [48-51] are prepared in Basic Language. They are given in Appendix I. The only difference between these two computer programs is in the compartment volumes. Whereas the first computer program is based on the initial compartment volumes given by Mackay et al [49], the second one is based on the final compartment volumes given by Mackay et al [51]. Table 5.2.1 shows the comparison of the first and last compartment volumes. The aim in preparing the first one is to get the same results for Mackay's hypothetical solute as given by Mackay et al [49]. The results obtained for Mackay's hypothetical solute are just as given by Mackay et al [49] and validate the program. In this study the second computer program based on the final compartment volumes is used for calculations. Figure 5.2.1 is the flow sheet of the program.

5.2.2 A Specimen Calculation

As given in Table A.2.7, benzene has a molecular weight of 78.114 gr, a water solubility of 1790 g/m^3, a vapor pressure of 95.044 mm Hg and a log K_{ow} of 2.13, i.e. K_{ow} is 134.896.

By using Level I Fugacity Model, the physical chemical data is converted into fugacity capacities and the partitioning behaviour of the chemical is easily calculated.

TABLE 5.2.1 - The Comparison of the Initial and Final Compartment Volumes Given by Mackay et al [49,51]

Compartment	Volume (m^3)	
	FIRST VALUES	
Air	10^{10}	(1 km^2 area x 10 km height)
Soil	$9x10^3$	(30% area x 3 cm depth)
Water	$7x10^6$	(70% area x 10 m depth)
Biota	3.5	(Water volume x 0.5 ppm)
Suspended solids	35	(Water volume x 5 ppm)
Sediment	$2.1x10^4$	(70% area x 3 cm depth)
	LAST VALUES	
Air	$6x10^9$	(1 km^2 area x 6 km height)
Soil	$4.5x10^4$	(30% area x 15 cm depth)
Water	$7x10^6$	(70% area x 10 m depth)
Biota	7	(Water volume x 1 ppm)
Suspended solids	35	(Water volume x 5 ppm)
Sediment	$2.1x10^4$	(70% area x 3 cm depth)

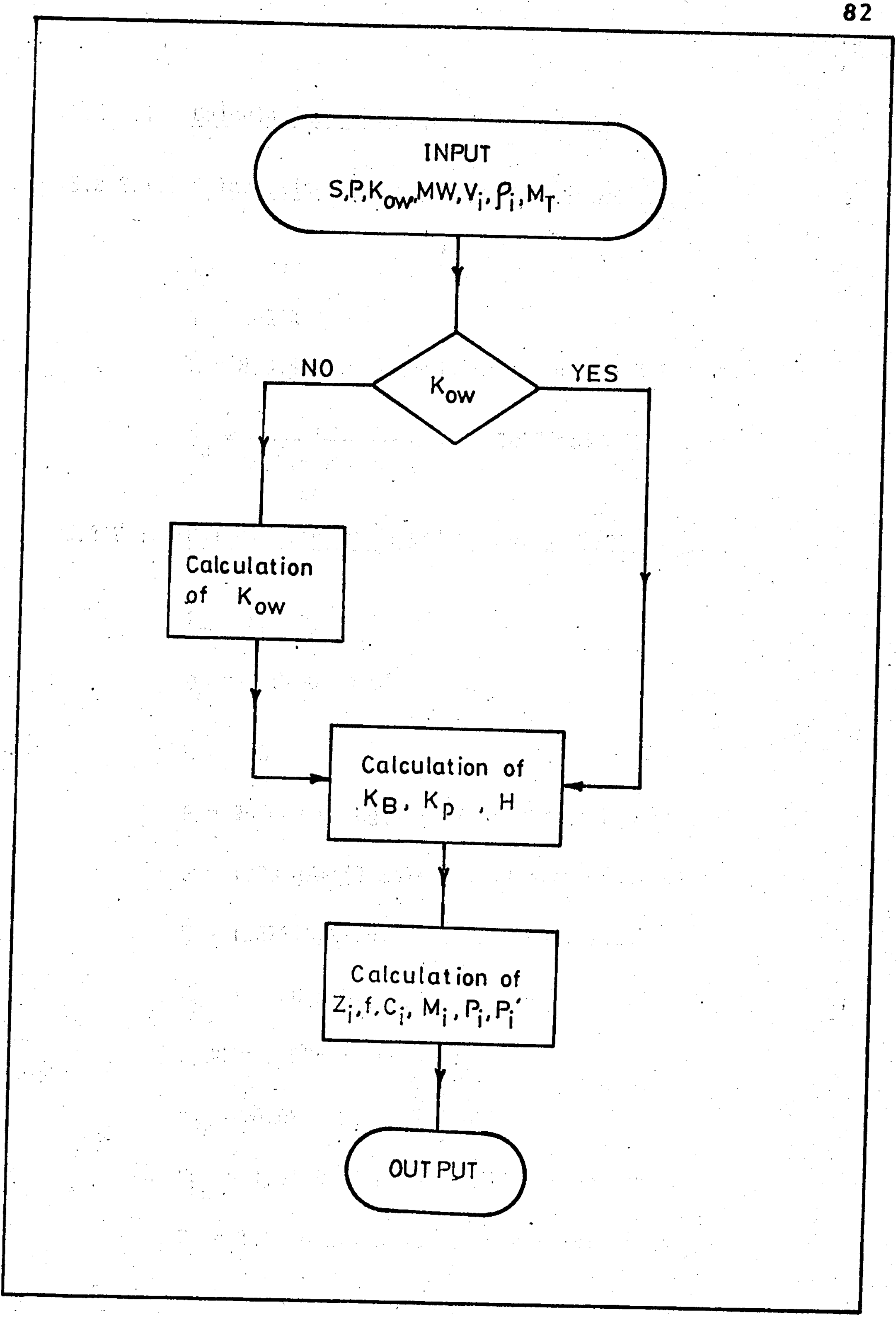


FIGURE 5.2.1. The flow sheet of the computer program

5.2.2.1 Calculation of Fugacity Capacities

5.2.2.1.1 Calculation of Fugacity Capacity for Air

$Z_a = 1/RT$

$T = 298°K$

$R = 8.314(\text{Pa.m}^3)/(\text{mol °K})$ or $8.314\ \text{J}/(\text{mol °K})$

$$Z_a = \frac{1}{8.314 \times 298} = 4.04\text{x}10^{-4}\ \text{mol/m}^3\text{Pa}$$

5.2.2.1.2 Calculation of Fugacity Capacity for Soil

$Z_s = K_{p_s}\ \rho_s/H$

$\rho_s = 1.5\text{x}10^6\ \text{g/m}^3$

$H = P/S$

$P = 95.044\ \text{mm Hg}(1\ \text{Pa}/7.5\text{x}10^{-3}\ \text{mm Hg}) = 12672.5\ \text{Pa}$

$S = 1790\ \text{g/m}^3(1\ \text{mole}/78.114\ \text{gram}) = 22.915\ \text{mole/m}^3$

$H = 12672.5/22.915 = 553.02\ \text{Pa m}^3/\text{mol}$

$K_{p_s} = \%\ \text{OC} \times 0.6 \times K_{ow}$

$\%\ \text{OC} = 0.02$ for soil

$K_{p_s} = 0.02 \times 0.6 \times 134.896$

$K_{p_s} = 1.6188\ \text{m}^3$ of water$/10^6$ g sorbent

$Z_s = 1.6188 \times 1.5/553.02 = 4.391\text{x}10^{-3}\ \text{mole/m}^3\ \text{Pa}$

5.2.2.1.3 Calculation of Fugacity Capacity for Water

$Z_W = 1/H$

$H = 553.02$ Pa m^3/mole

$Z_W = 1/553.02 = 1.808\times10^{-3}$ mole/m^{3}Pa

5.2.2.1.4 Calculation of Fugacity Capacity for Biota

$Z_b = K_B \rho_b / H$

$\rho_b = 1\times10^6$ g/m^3

$H = 553.02$ Pa m^3/mole

$\log K_B = 0.85 \log K_{ow} - 0.7$

$\log K_B = 0.85 \times 2.13 - 0.7$

$\log K_B = 1.1105$

$K_B = 12.897$ m^3 of water/10^6 g biota

$Z_b = (12.897 \times 1)/553.02 = 2.332\times10^{-2}$ mole/m^{3}Pa

5.2.2.1.5 Calculation of Fugacity Capacity for Suspended Solids

$Z_{ss} = K_{p_{ss}} \rho_{ss}/H$

$\rho_{ss} = 1.5\times10^6$ g/m^3

$H = 553.02$ Pa m^3/mole

$K_{p_{ss}} = \%\ OC \times 0.6 \times K_{ow}$

% OC = 0.04 for suspended solids

$K_{p_{ss}} = 0.04 \times 0.6 \times 134.896$

$K_{p_{ss}} = 3.2375$ m^3 of water/10^6 g sorbent

$Z_{ss} = (3.2375 \times 1.5)/553.02 = 8.781\times10^{-3}$ mole/m^{3}Pa

5.2.2.1.6 Calculation of Fugacity Capacity for Sediment

$Z_{sd} = K_{p_{sd}}\ \rho_{sd}/H$

$\rho_{sd} = 1.5\times10^6$ g/m^3

$H = 553.02$ m^{3}Pa/mole

$K_{p_{sd}} = \%\ OC \times 0.6 \times K_{ow}$

% OC = 0.04 for sediment

$K_{p_{sd}} = 0.04 \times 0.6 \times 134.896$

$K_{p_{sd}} = 3.2375$ m^3 of water/10^6 g sorbent

$Z_{sd} = (3.2375 \times 1.5)/553.02 = 8.781\times10^{-3}$ mole/m^{3}Pa

5.2.2.2 Calculation of Prevailing Common Fugacity

$f = M_T/\Sigma Z_i V_i$

$M_T = 100$ mole

$Z_a = 4.04\times10^{-4}$ mole/m^{3}Pa

$V_a = 6\times10^9$ m^3

$Z_aV_a = (4.04\text{x}10^{-4})(6\text{x}10^{9}) = 24.23\text{x}10^{5}$ mole/Pa

$Z_s = 4.391\text{x}10^{-3}$ mole/m^{3}Pa

$V_s = 4.5\text{x}10^{4}$ m^3

$Z_sV_s = (4.391\text{x}10^{-3})(4.5\text{x}10^{4}) = 197.6$ mole/Pa

$Z_w = 1.808\text{x}10^{-3}$ mole/m^{3}Pa

$V_w = 7\text{x}10^{6}$ m^3

$Z_wV_w = (1.808\text{x}10^{-3})(7\text{x}10^{6}) = 12\,656$ mole/Pa

$Z_b = 2.332\text{x}10^{-2}$ mole/m^{3}Pa

$V_b = 7$ m^3

$Z_bV_b = (2.332\text{x}10^{-2})(7) = 0.1632$ mole/Pa

$Z_{ss} = 8.781\text{x}10^{-3}$ mole/m^{3}Pa

$V_{ss} = 35$ m^3

$Z_{ss}V_{ss} = (8.781\text{x}10^{-3})(35) = 0.3073$ mole/Pa

$Z_{sd} = 8.781\text{x}10^{-3}$ mole/m^{3}Pa

$V_{sd} = 2.1\text{x}10^{4}$ m^3

$Z_{sd}V_{sd} = (8.781\text{x}10^{-3})(2.1\text{x}10^{4}) = 184.401$ mole/Pa

$\Sigma Z_iV_i = Z_aV_a + Z_sV_s + Z_wV_w + Z_bV_b + Z_{ss}V_{ss} + Z_{sd}V_{sd}$

$\Sigma Z_iV_i = (24.23\text{x}10^{5}) + 197.6 + 12656 + 0.1632 + 0.3073 + 184.401$

$\Sigma Z_iV_i = 2.44\text{x}10^{6}$ mole/Pa

$f = M_T/\Sigma Z_i V_i = 100/(2.44\times10^{6}) = 4.105\times10^{-5}$ Pa

5.2.2.3 Calculation of Amounts

$M_i = f\ Z_i\ V_i$

$f = 4.105\times10^{-5}$ Pa

$M_a = f\ Z_a\ V_a$

$Z_aV_a = 24.23\times10^{5}$ mole/Pa

$M_a = (4.105\times10^{-5})(24.23\times10^{5}) = 99.464$ mole

$M_s = f\ Z_sV_s$

$Z_sV_s = 197.6$ mole/Pa

$M_s = (4.105\times10^{-5})(197.6) = 8.111\times10^{-3}$ mole

$M_w = f\ Z_wV_w$

$Z_wV_w = 12656$ mole/Pa

$M_w = (4.105\times10^{-5})(12656) = 0.5195$ mole

$M_b = f\ Z_bV_b$

$Z_bV_b = 0.1632$ mole/Pa

$M_b = (4.105\times10^{-5})(0.1632) = 6.699\times10^{-6}$ mole

$M_{ss} = f\ Z_{ss}V_{ss}$

$Z_{ss}V_{ss} = 0.3073$ mole/Pa

$M_{ss} = (4.105\times10^{-5})(0.3073) = 1.261\times10^{-5}$ mole

$M_{sd} = f\ Z_{sd}V_{sd}$

$Z_{sd}V_{sd} = 184.40$ mole/Pa

$M_{sd} = (4.105\text{x}10^{-5})(184.40) = 7.570\text{x}10^{-3}$ mole

5.2.2.4 Calculation of Concentrations

$C_i = f\ Z_i$

$f = 4.105\text{x}10^{-5}$ Pa

$C_a = f\ Z_a$

$Z_a = 4.04\text{x}10^{-4}$ mole/m³Pa

$C_a = (4.105\text{x}10^{-5})(4.04\text{x}10^{-4}) = 1.658\text{x}10^{-8}$ mole/m³

$$C_a = (1.658\text{x}10^{-8} \text{ mole/m}^3)(78.114 \text{ gr/1 mole})(1\ \mu\text{g}/10^{-6} \text{ g})$$
$$\text{x } (1 \text{ m}^3 \text{ air}/1.19\text{x}10^3 \text{ gr})$$

$C_a = 1.088\text{x}10^{-3}\ \mu$g/g or ppm

$C_s = f\ Z_s$

$Z_s = 4.391\text{x}10^{-3}$ mole/m³Pa

$C_s = (4.105\text{x}10^{-5})(4.391\text{x}10^{-3}) = 1.803\text{x}10^{-7}$ mole/m³

$$C_s = (1.803\text{x}10^{-7} \text{ mole/m}^3)(78.114 \text{ g/1 mole})(1\ \mu\text{g}/10^{-6} \text{ g})$$
$$\text{x } (1 \text{ m}^3 \text{ soil}/1.5\text{x}10^6 \text{ g})$$

$C_s = 9.389\text{x}10^{-6}\ \mu$g/g or ppm

$C_w = f\ Z_w$

$Z_w = 1.808\text{x}10^{-3}$ mole/m^{3}Pa

$C_w = (4.105\text{x}10^{-5})(1.808\text{x}10^{-3}) = 7.422\text{x}10^{-8}$ mole/m^3

$C_w = (7.442\text{x}10^{-8}$ mole/m^3)(78.114 g/1 mole)(1 μg/10^{-6} g)

x (1 m^3 water/1x10^6 g)

$C_w = 5.797\text{x}10^{-6}$ μg/g or ppm

$C_b = f\ Z_b$

$Z_b = 2.332\text{x}10^{-2}$ mole/m^{3}Pa

$C_b = (4.105\text{x}10^{-5})(2.332\text{x}10^{-2}) = 9.573\text{x}10^{-7}$ mole/m^3

$C_b = (9.573\text{x}10^{-7}$ mole/m^3)(78.114 gr/1 mole)(1 μg/10^{-6} g)

x (1 m^3 biota/1x10^6 g)

$C_b = 7.478\text{x}10^{-5}$ μg/g or ppm

$C_{ss} = f\ Z_{ss}$

$Z_{ss} = 8.781\text{x}10^{-3}$ mole/m^{3}Pa

$C_{ss} = (4.105\text{x}10^{-5})(8.781\text{x}10^{-3}) = 3.605\text{x}10^{-7}$ mole/m^3

$C_{ss} = (3.605\text{x}10^{-7}$ mole/m^3)(78.114 g/1 mole)(1 μg/10^{-6} g)

x (1 m^3 susp.sol./1.5x10^6 g)

$C_{ss} = 1.877\text{x}10^{-5}$ μg/g or ppm

$C_{sd} = f\ Z_{sd}$

$Z_{sd} = 8.781\text{x}10^{-3}$ mole/m^{3}Pa

$C_{sd} = (4.105\text{x}10^{-5})(8.781\text{x}10^{-3}) = 3.605\text{x}10^{-7}$ mole/m^3

$C_{sd} = (3.605\text{x}10^{-7}$ mole/m^3)(78.114 g/1 mole)(1 μg/10^{-6} g)

x (1 m^3 sediment/1.5x10^6 g)

$C_{sd} = 1.877\text{x}10^{-5}$μg/g or ppm

5.2.2.5 Calculation of Mass Partitioning

$P_i = Z_iV_i/\Sigma Z_iV_i$

$\Sigma Z_iV_i = Z_aV_a + Z_sV_s + Z_wV_w + Z_bV_b + Z_{ss}V_{ss} + Z_{sd}V_{sd}$

$\Sigma Z_iV_i = 24.23\text{x}10^5 + 197.6 + 12656 + 0.1632 + 0.3073 + 184.4$

$\Sigma Z_iV_i = 2.44\text{x}10^6$ mole/Pa

$P_a = Z_aV_a/\Sigma Z_iV_i$

$Z_aV_a = 24.23\text{x}10^5$ mole/Pa

$P_a = 24.23\text{x}10^5/2.44\text{x}10^6 = 0.9930$

$P_s = Z_sV_s/\Sigma Z_iV_i$

$Z_sV_s = 197.6$ mole/Pa

$P_s = 197.6/2.44\text{x}10^6 = 8.098\text{x}10^{-5}$

$P_w = Z_w V_w / \Sigma Z_i V_i$

$Z_w V_w = 12656$ mole/Pa

$P_w = 12656/2.44\times10^{6} = 5.187\times10^{-3}$

$P_b = Z_b V_b / \Sigma Z_i V_i$

$Z_b V_b = 0.1632$ mole/Pa

$P_b = 0.1632/2.44\times10^{6} = 6.688\times10^{-8}$

$P_{ss} = Z_{ss} V_{ss} / \Sigma Z_i V_i$

$Z_{ss} V_{ss} = 0.3073$ mole/Pa

$P_{ss} = 0.3073/2.44\times10^{6} = 1.259\times10^{-7}$

$P_{sd} = Z_{sd} V_{sd} / \Sigma Z_i V_i$

$Z_{sd} V_{sd} = 184.4$ mole/Pa

$P_{sd} = 184.4/2.44\times10^{6} = 7.557\times10^{-5}$

5.2.2.6 Calculation of Equilibrium Partitioning

$P_i^! = Z_i / \Sigma Z_i$

$\Sigma Z_i = Z_a + Z_s + Z_w + Z_b + Z_{ss} + Z_{sd}$

$$\Sigma Z_i = (4.04\times10^{-4}) + (4.391\times10^{-3}) + (1.808\times10^{-3}) + (2.332\times10^{-2}) + (8.781\times10^{-3}) + (8.781\times10^{-3})$$

$\Sigma Z_i = 47.485\times10^{-3}$

$P'_a = Z_a/\Sigma Z_i$

$P'_a = 4.04\times10^{-4}/47.485\times10^{-3} = 85.079\times10^{-4}$

$P'_s = Z_s/\Sigma Z_i$

$P'_s = 4.391\times10^{-3}/47.485\times10^{-3} = 9.248\times10^{-2}$

$P'_w = Z_w/\Sigma Z_i$

$P'_w = 1.808\times10^{-3}/47.485\times10^{-3} = 3.808\times10^{-2}$

$P'_b = Z_b/\Sigma Z_i$

$P'_b = 2.332\times10^{-2}/47.485\times10^{-3} = 0.4911$

$P'_{ss} = Z_{ss}/\Sigma Z_i$

$P'_{ss} = 8.781\times10^{-3}/47.485\times10^{-3} = 0.1849$

$P'_{sd} = Z_{sd}/\Sigma Z_i$

$P'_{sd} = 8.781\times10^{-3}/47.485\times10^{-3} = 0.1849$

The results are listed in Table 5.2.2 which shows that 99% of benzene partitions into air compartment, thus the amounts in the other compartments are unimportant. Because the amount in the air compartment is greater than 90%, there is a need for further studies on degradation in the air compartment according to Neely's decision tree given in Figure 4.1.1.

TABLE 5.2.2 - Calculated Equilibrium Distribution of Benzene

Name of Chemical	MW g/gmole	P mm Hg	S g/m^3	$\log K_{ow}$
Benzene	78.114	95.044	1790	2.13

Compartment	Mass Part.	Equi. Part.	Amount (mole)	Concentration (ppm)
Air	0.9930	85.08×10^{-4}	99.464	1.09×10^{-3}
Soil	8.10×10^{-5}	9.25×10^{-2}	8.11×10^{-3}	9.39×10^{-6}
Water	5.19×10^{-3}	3.81×10^{-2}	0.5195	5.8×10^{-6}
Biota	6.69×10^{-7}	0.4911	6.7×10^{-6}	7.48×10^{-5}
Suspended Solids	1.26×10^{-7}	0.1849	1.26×10^{-5}	1.88×10^{-5}
Sediment	7.56×10^{-5}	0.1849	7.57×10^{-3}	1.88×10^{-5}

5.3 RESULTS AND DISCUSSION

The outputs given in Appendix I are arranged in order of forming several families such as monosubstituted benzene family, halobenzene family, toluene family, phenol family, aniline family and nitrobenzene family and their partitioning behaviour between the environmental compartments are discussed here.

Monosubstituted benzenes partition either into the air compartment or into the water compartment depending upon the substituted group on the benzene ring. Benzene, mono alkyl benzenes except butylbenzene, monohalobenzenes mostly partition into the air compartment as illustrated in Figure 5.3.1 and Figure 5.3.3. Since their mass percentages in that compartment are greater than 90 percent, they are significant for the air compartment according to the Neely's decision tree. Butylbenzene, benzyl alcohol, phenol, anisole, aniline, N-N-dimethyl aniline, acetophenone and nitrobenzene mostly partition into the water compartment. As illustrated in Figure 5.3.2 and Figure 5.3.4, since their mass percentages in that compartment are much greater than two percent, they are important for the water compartment according to the Neely's decision tree [2].

Although 99 percent of monoalkylbenzenes except butylbenzene partitions into the air compartment, only 57.19 percent of butylbenzene partitions into that compartment as illustrated in Figure 5.3.5. It can be seen in Figure 5.3.6 that 41.99 percent of butylbenzene goes to the water compartment. Whereas this compound is not significant for the air compartment as its mass percentage in that compartment is less than

THE BENZENE FAMILY SUBSTITUTED FOR AN ELECTRON-RELEASING GROUP IN THE AIR COMPARTMENT

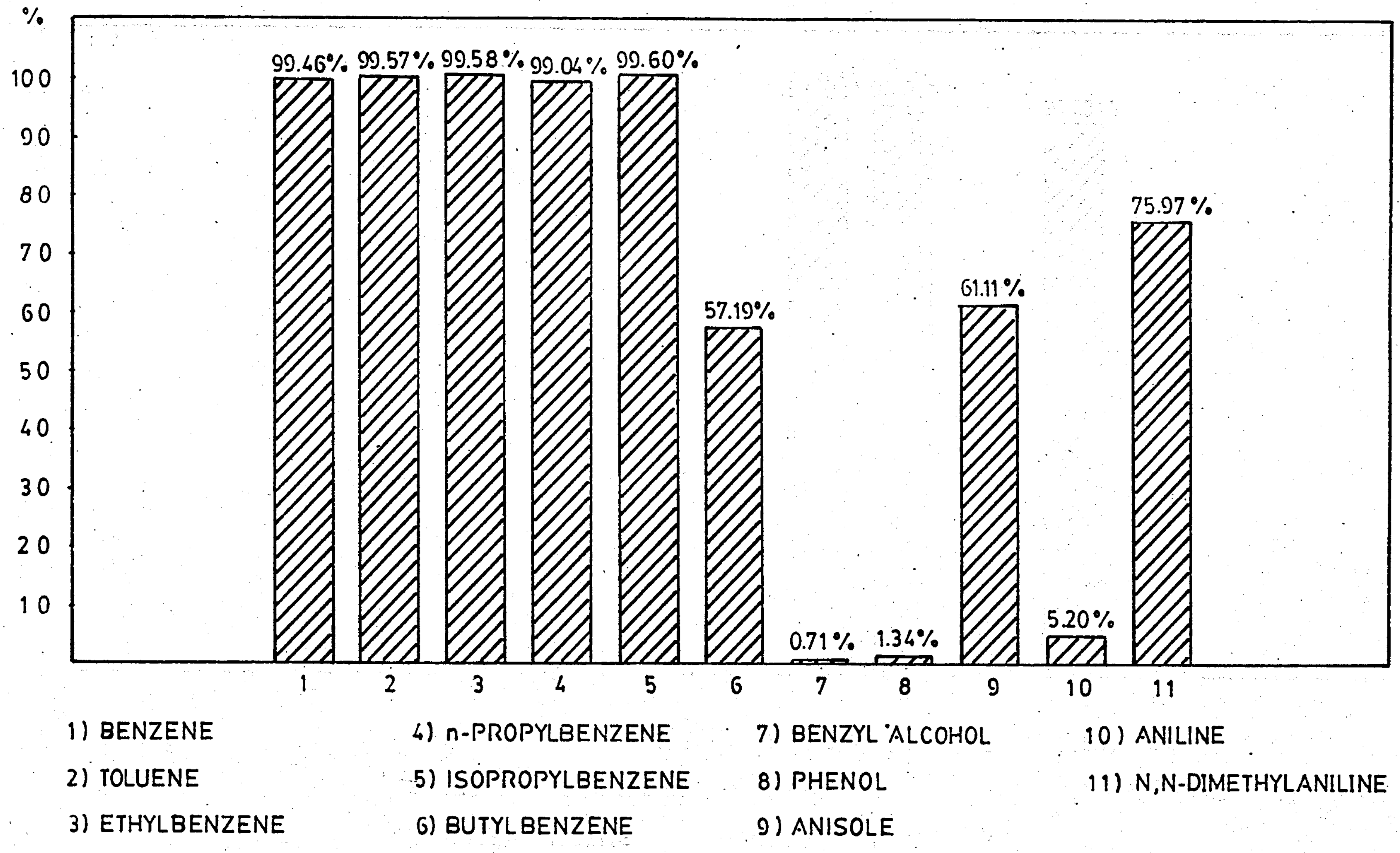


FIGURE 5.3.1 The bargraph of benzene family substituted for an electron-releasing group in the air compartment

THE BENZENE FAMILY SUBSTITUTED FOR AN ELECTRON-RELEASING GROUP IN THE WATER COMPARTMENT

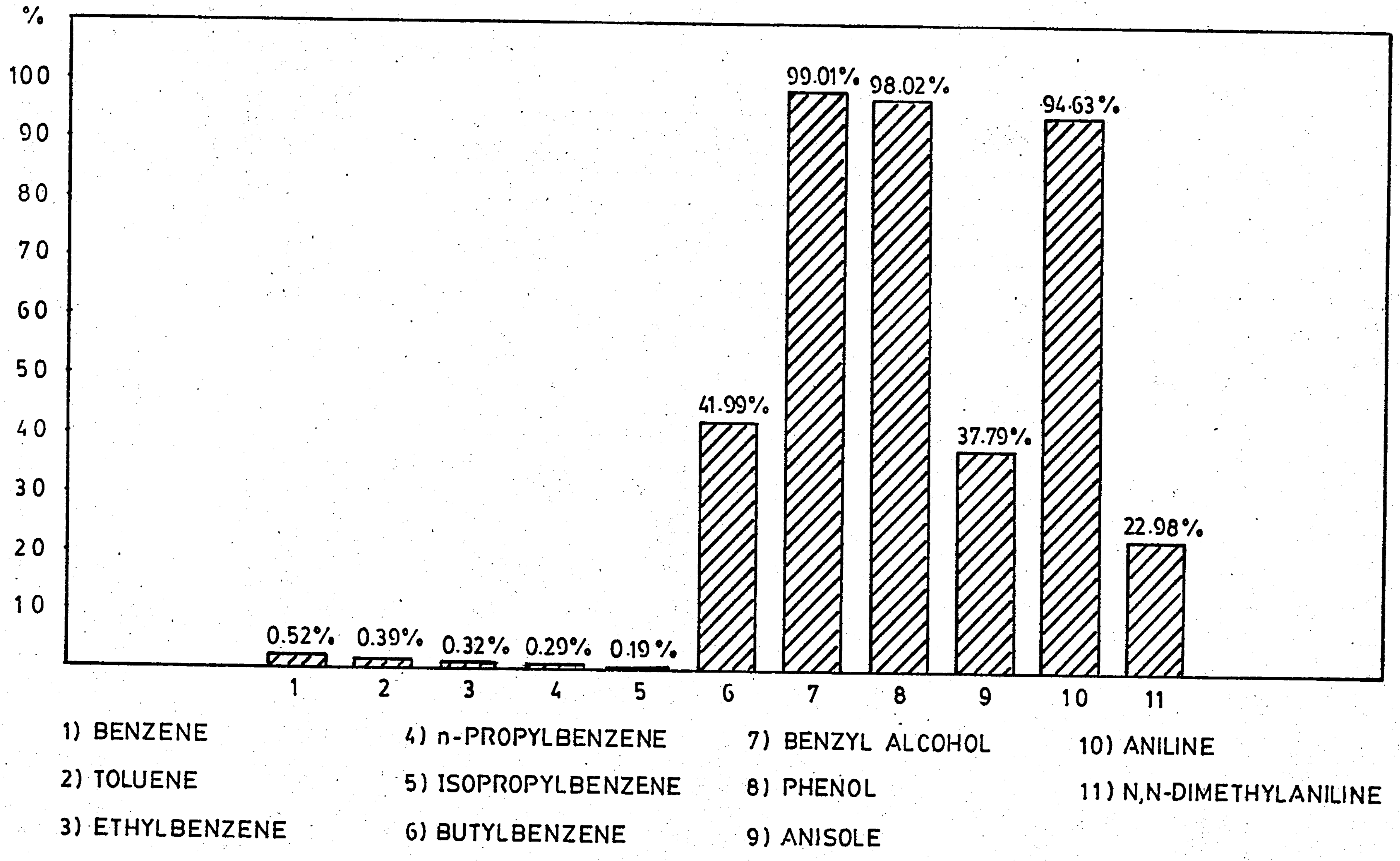
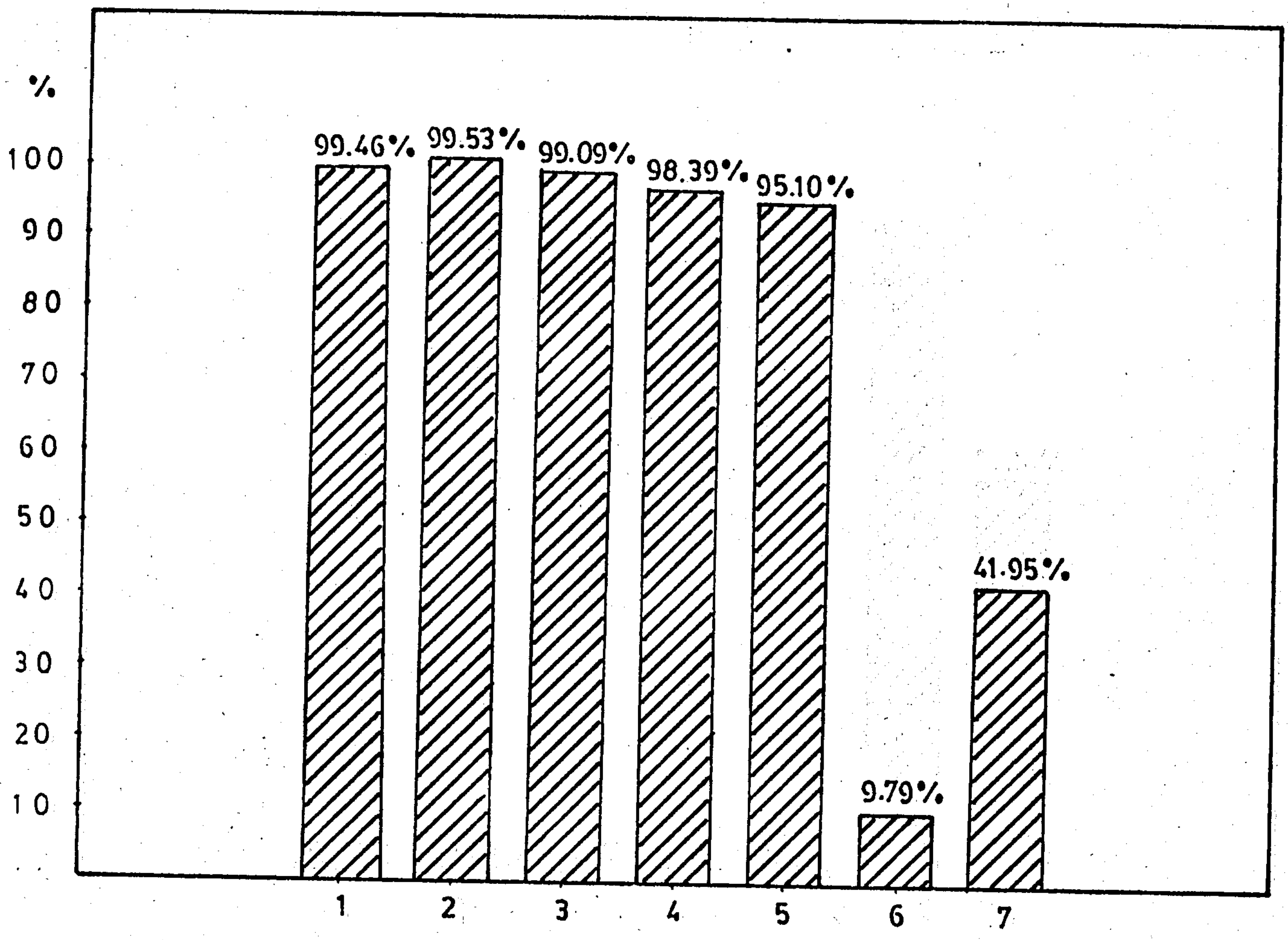


FIGURE 5.3.2. The bargraph of benzene family substituted for an electron-releasing group in the water compartment

THE BENZENE FAMILY SUBSTITUTED FOR AN ELECTRON-WITHDRAWING GROUP IN THE AIR COMPARTMENT



1) BENZENE
2) FLUOROBENZENE
3) CHLOROBENZENE
4) BROMOBENZENE
5) IODOBENZENE
6) ACETOPHENONE
7) NITROBENZENE

FIGURE 5.3.3. The bargraph of benzene family substituted for an electron-withdrawing group in the air compartment

THE BENZENE FAMILY SUBSTITUTED FOR AN ELECTRON-WITHDRAWING GROUP IN THE WATER COMPARTMENT

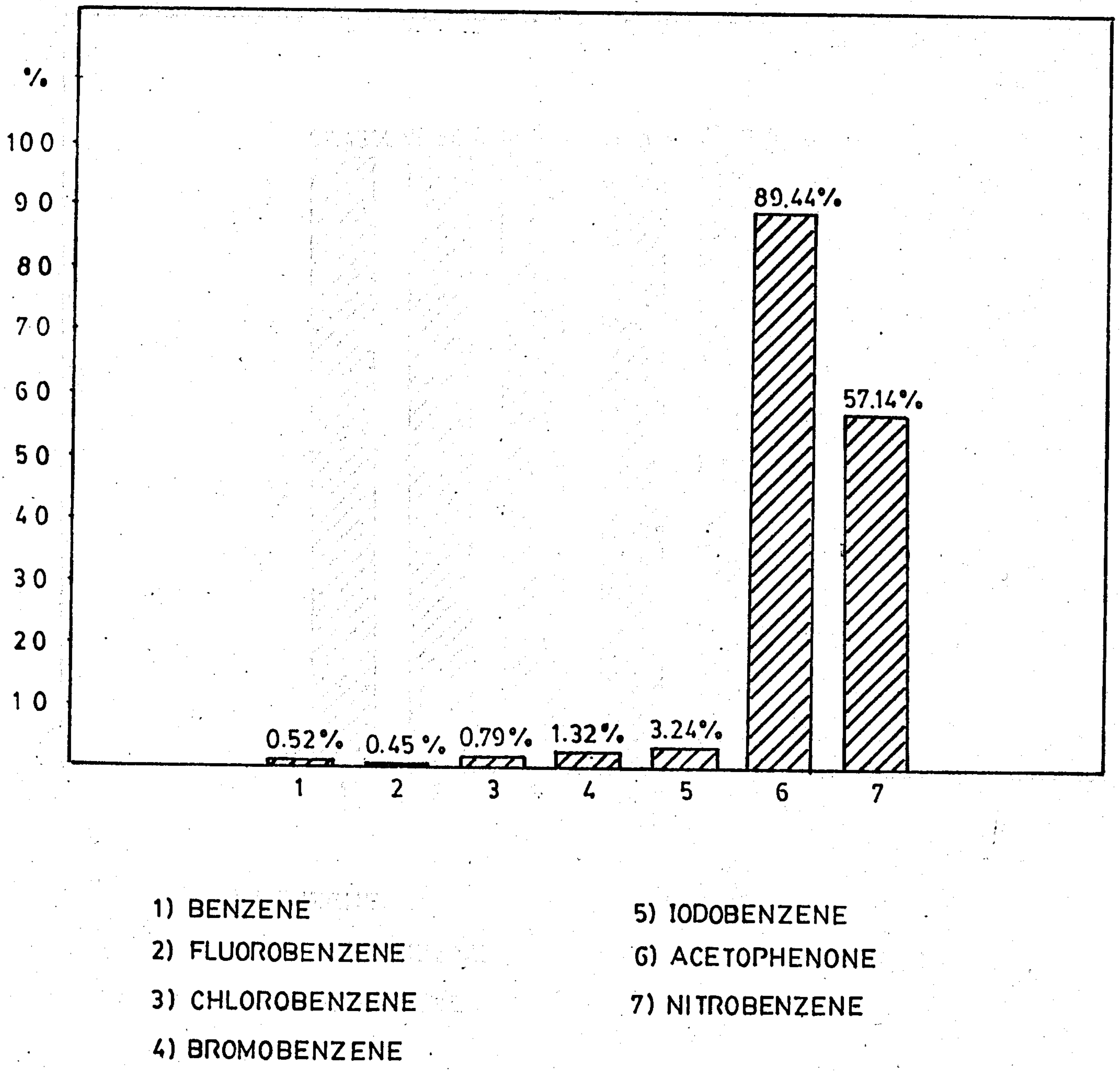


FIGURE 5.3.4 The bargraph of benzene family substituted for an electron-withdrawing group in the water compartment

THE ALKYLBENZENE FAMILY IN THE AIR COMPARTMENT

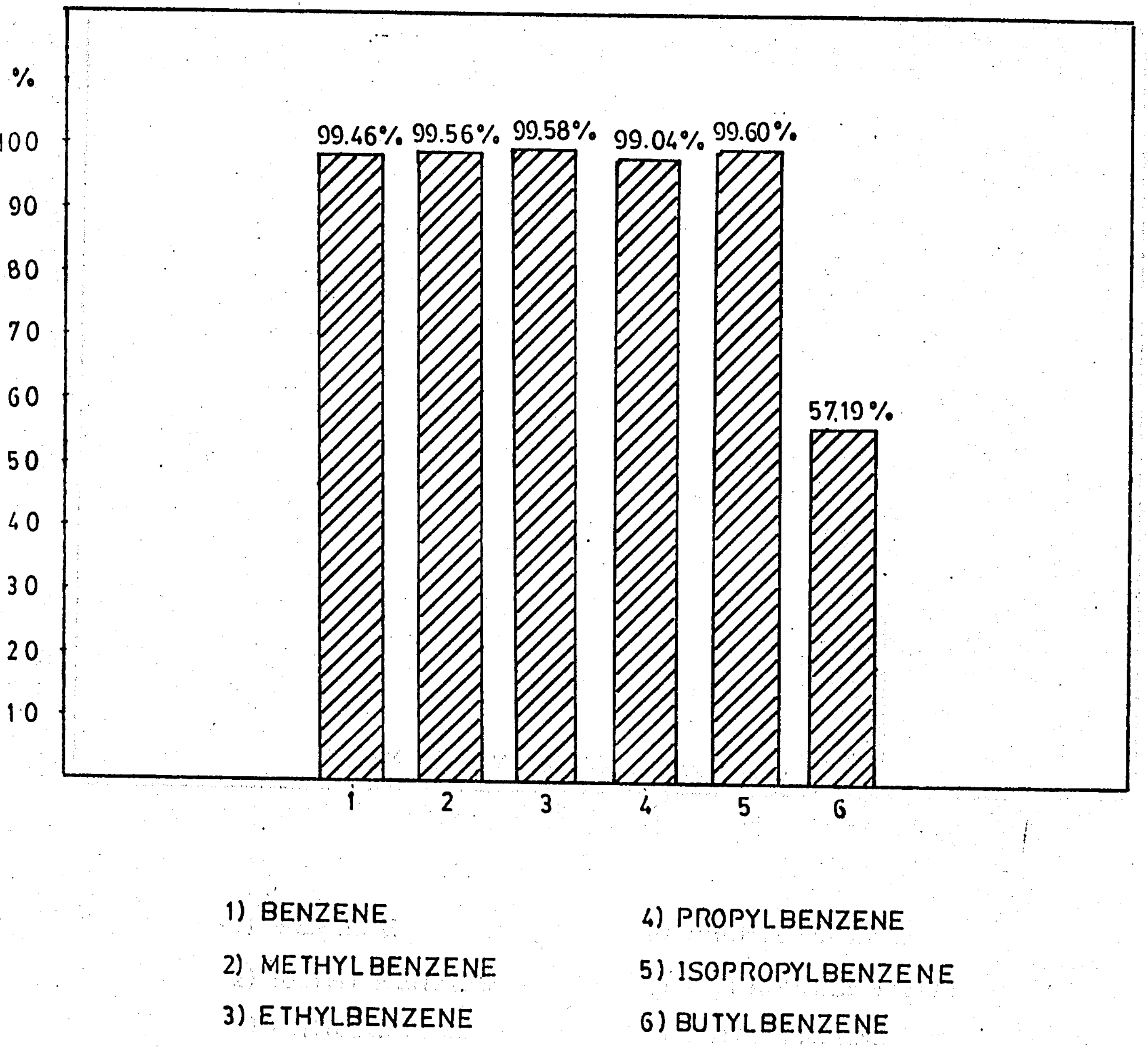


FIGURE 5.3.5 The bargraph of the alkylbenzene family in the air compartment

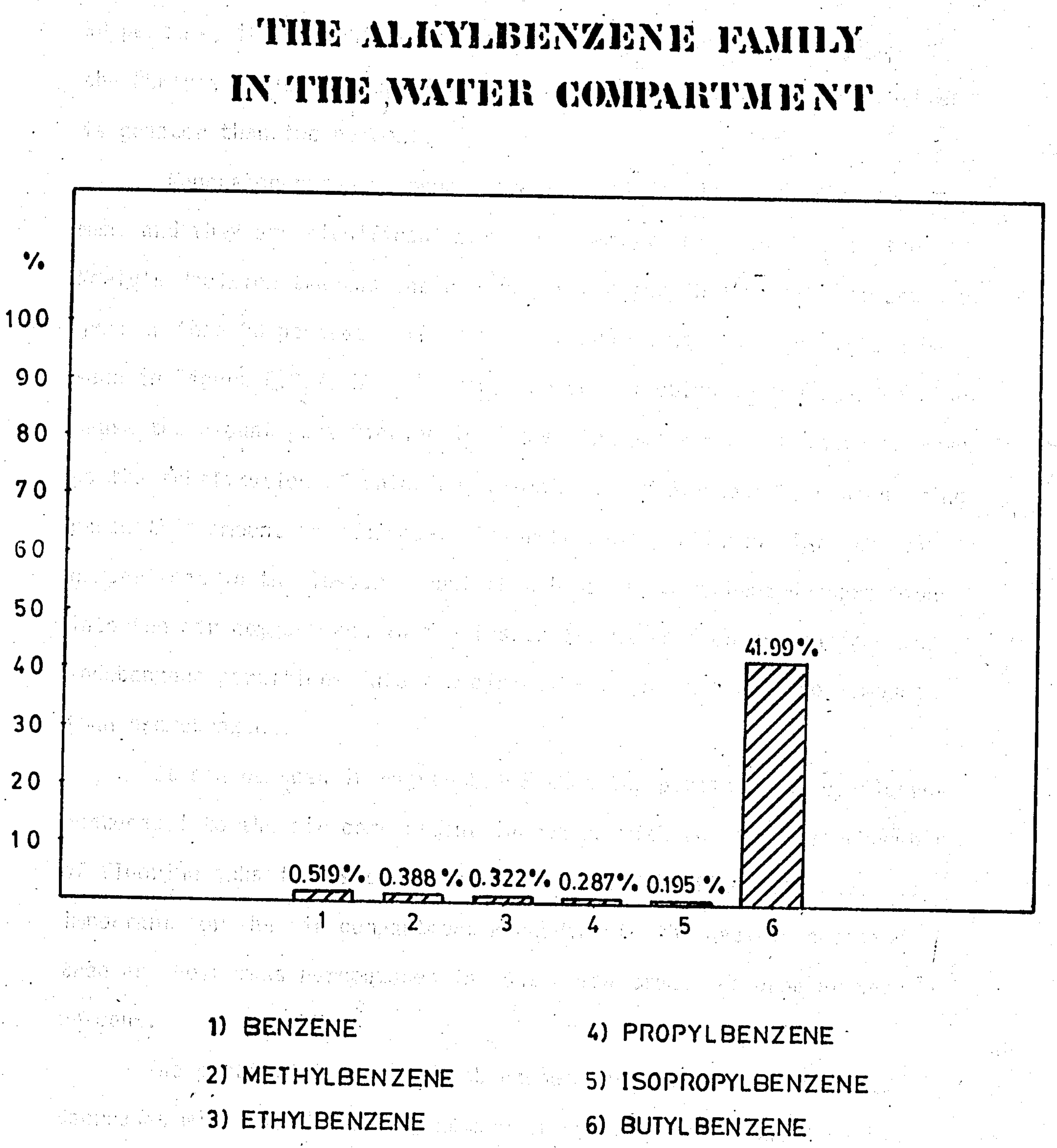


FIGURE 5.3.6. The bargraph of the alkylbenzene family in the water compartment

90 percent, it is significant for the water compartment according to the Neely's decision tree since its mass percentage in that compartment is greater than two percent.

Monohalogenated benzenes mostly partition into the air compartment and they are significant for this compartment according to the Neely's decision tree as their mass percentages in that compartment are greater than 90 percent. If they are compared with benzene it can be seen in Figure 5.3.7 that the fluorine substitution on the benzene ring cause the amount partitioning into the air compartment to increase whereas the substitution of chlorine, bromine and iodine on the benzene ring cause this amount to decrease. Chlorobenzene partitions into the air compartment in the lesser amount than benzene, bromobenzene partitions into the air compartment in the lesser amount than chlorobenzene, and iodobenzene partitions into the air compartment in the lesser amount than bromobenzene.

It can be seen in Figure 5.3.8 that the partitioning of fluorobenzenes into the air compartment increases with the increasing number of fluorine substitutes on the benzene ring. All fluorobenzenes are important for the air compartment according to the Neely's decision tree as their mass percentages in that compartment are greater than 90 percent.

The partitioning of chlorobenzenes into the air compartment decreases with the increasing number of chlorine substitutes on the benzene ring as illustrated in Figure 5.3.9. For hexachlorobenzene the amount that partitions into the air compartment is reduced to 58.28 percent and thus hexachlorobenzene becomes insignificant for the air

THE MONOHALOBENZENE FAMILY IN THE AIR COMPARTMENT

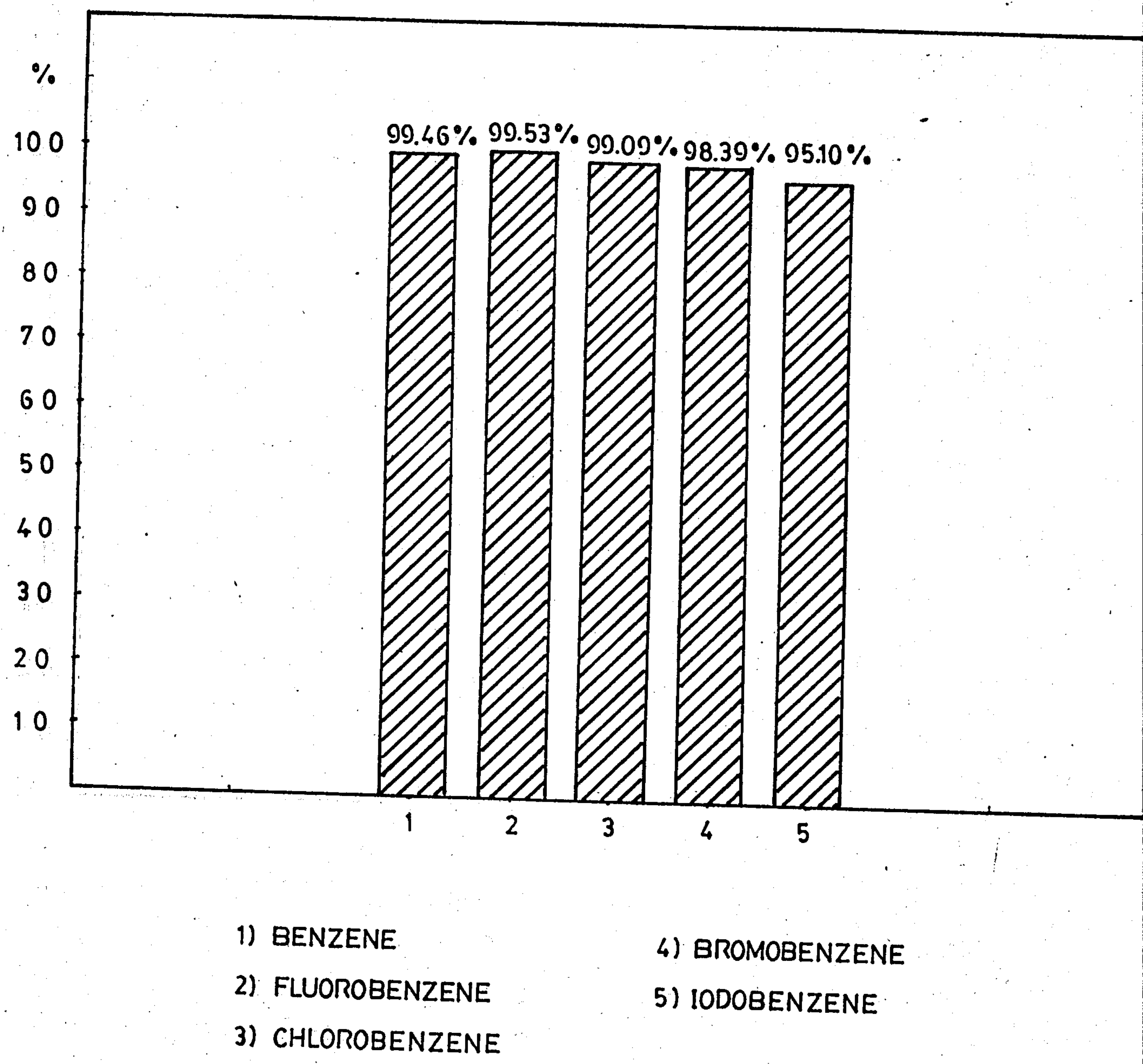


FIGURE 5.3.7. The bargraph of the monohalobenzene family in the air compartment

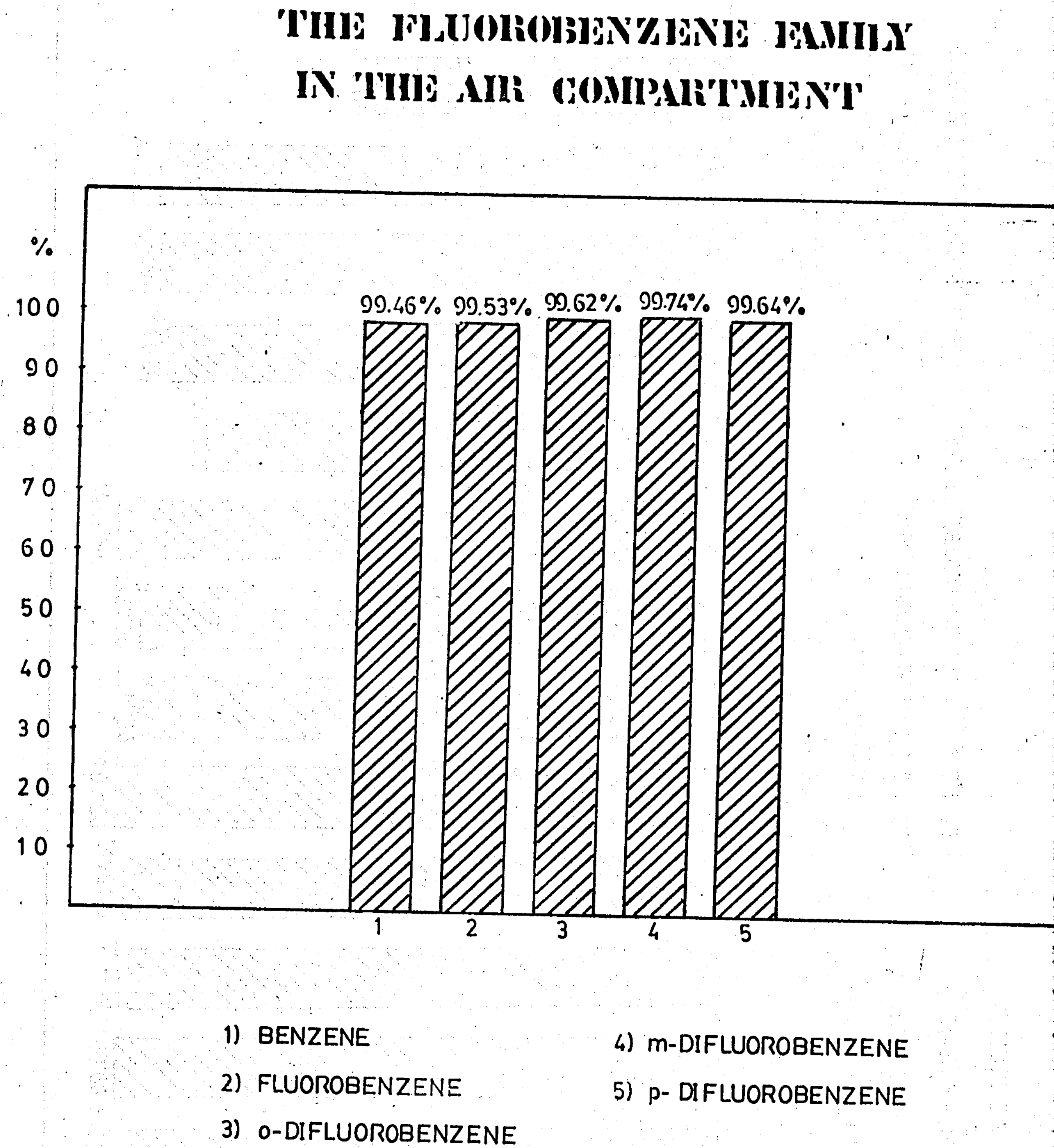


FIGURE 5.3.8. The bargraph of the fluorobenzene family in the air compartment

THE CHLOROBENZENE FAMILY IN THE AIR COMPARTMENT

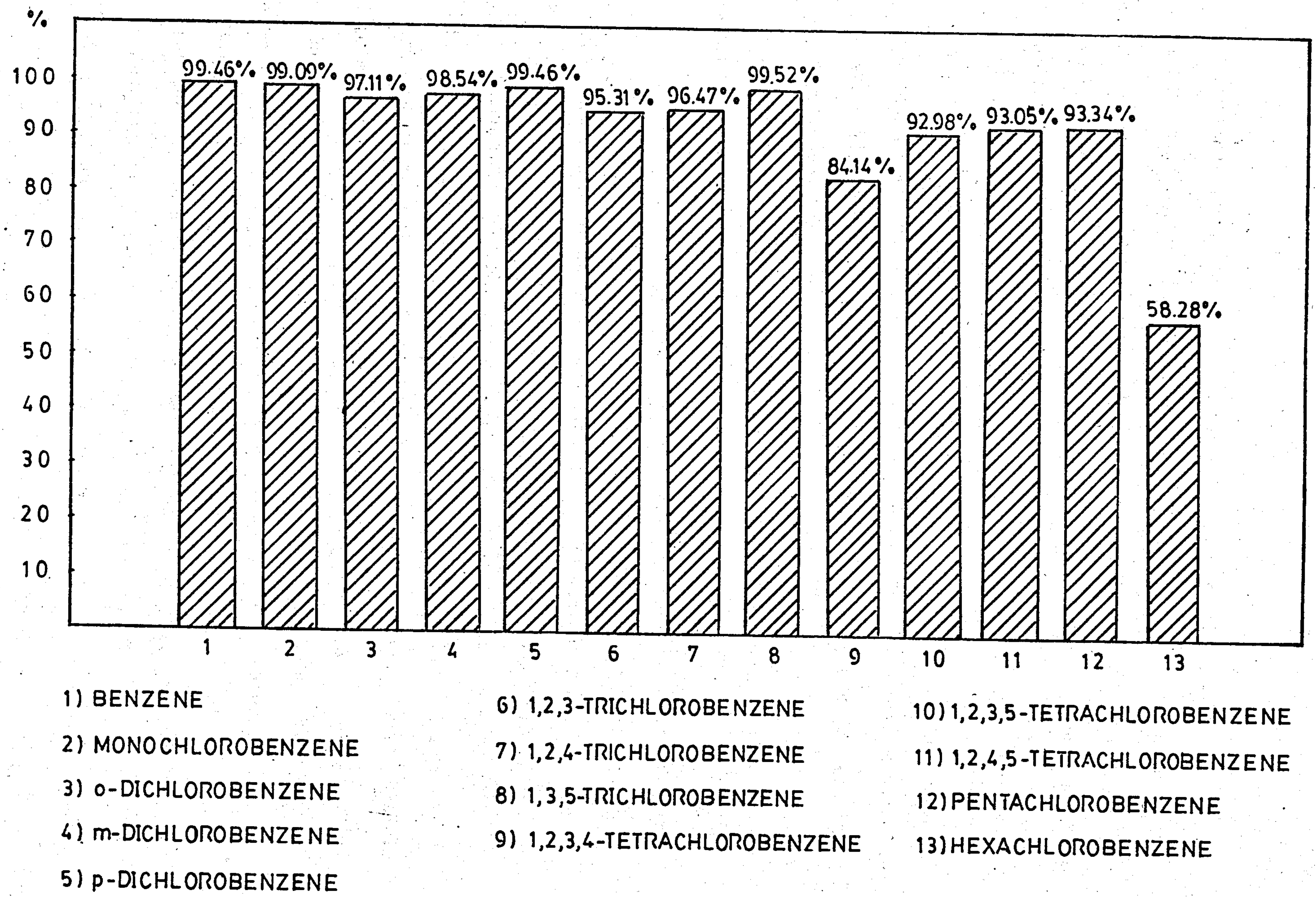


FIGURE 5.3.9. The bargraph of chlorobenzene family in the air compartment

compartment according to the Neely's decision tree since its amount in that compartment is less than 90 percent. 1, 2, 3, 4-tetrachlorobenzene partitions into the air compartment in the lesser amount than other two tetrachlorobenzenes. It is possible to say that this compound is insignificant for the air compartment according to the Neely's decision tree, since the amount partitioning into the air compartment is not greater than 90 percent. On the other hand, this amount is near 90 percent, it can be thought that this compound might be important for the air compartment. All the other chlorinated benzenes except hexachlorobenzene and 1,2,3,4-tetrachlorobenzene are significant for the air compartment since their mass percentages in that compartment is greater than 90 percent.

It can be seen in Figure 5.3.10 that the partitionings of chlorobenzenes into the soil and sediment compartments increase with the increasing number of chlorine substitutes on the benzene ring. Tetrachlorobenzenes, pentachlorobenzene, and hexachlorobenzene significantly partition into the soil and sediment compartments. The amounts of 1,2,3,4-tetrachlorobenzene that partition into these two compartments are greater than those of other two tetrachlorobenzenes. It is possible to say according to the Neely's decision tree that 1,2,3,4-tetrachlorobenzene is important for the soil and sediment compartments since its amounts partitioning into these two compartments are greater than four percent. It is also possible to say according to the Neely's decision tree that the other two tetrachlorobenzenes and pentachlorobenzene are unimportant for these two compartments since their mass percentages are not greater than four percent. On the other hand it can be thought that

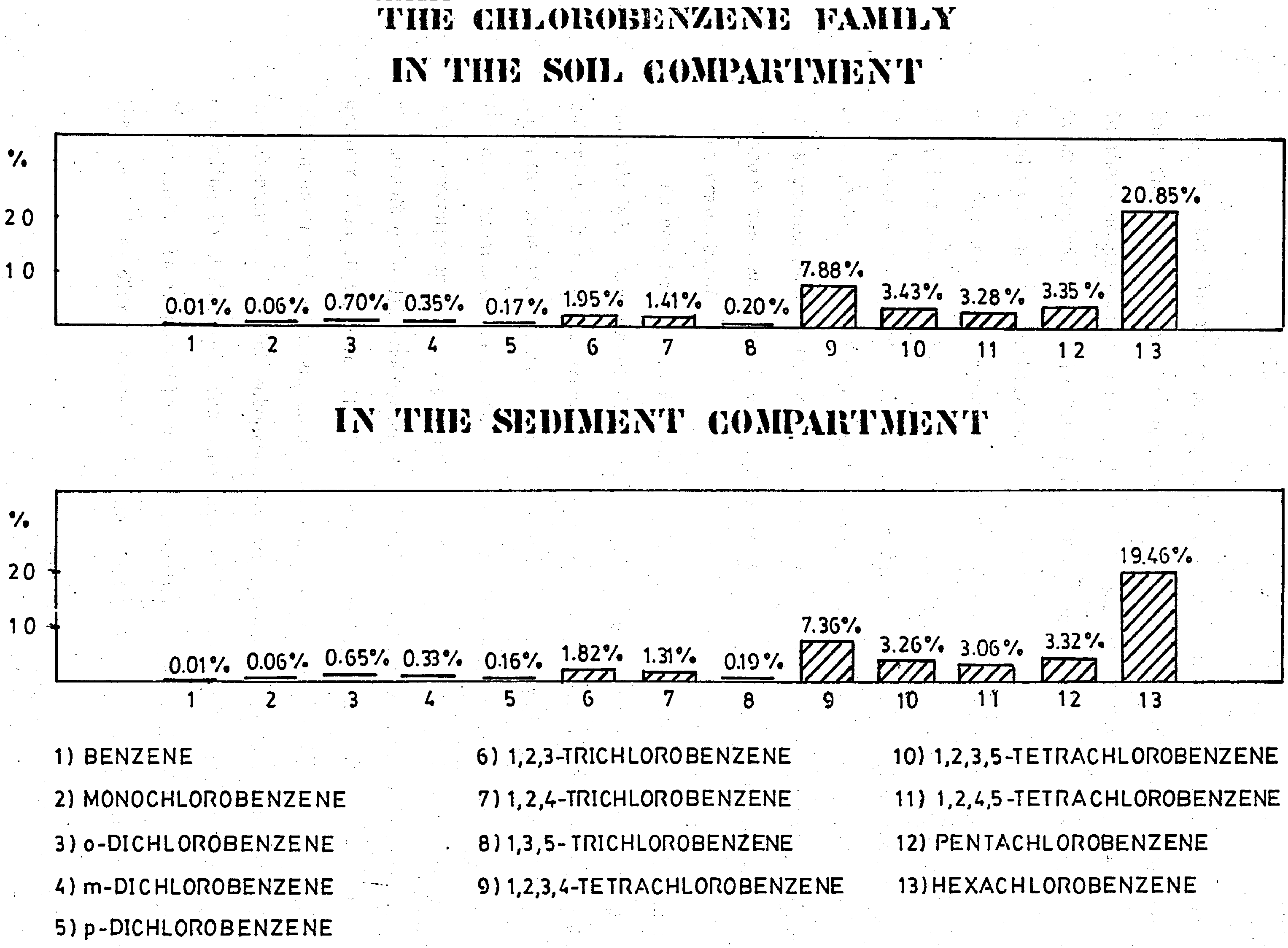


FIGURE 5.3.10. The bargraph of chlorobenzene family in the soil and sediment compartments

1,2,3,5-tetrachlorobenzene and 1,2,4,5-tetrachlorobenzene might be important for the soil and sediment compartments since their mass percentages in those compartments are near four percent. Hexachlorobenzene partitions more significantly into the soil and sediment compartments compared with the other chlorinated benzenes.

The compounds important for the soil and sediment compartments should be important for the suspended solids compartments. Although the biota and suspended solids compartments are insignificant from a mass balance point of view, higher concentrations are reached in these compartments than in the other compartments. Tetrachlorobenzenes, pentachlorobenzene and hexachlorobenzene reach high concentrations in the biota compartment.

As can be seen in Figure 5.3.11, the partitioning of bromobenzenes into the air compartment decrease with the increasing number of bromine substituents on the benzene ring significantly compared with those of the chlorine substituents and thus tribromobenzenes become insignificant for the air compartment according to the Neely's decision tree, since their mass percentages in that compartment is less than 90 percent. Although the amount of p-dibromobenzene partitioning into the air compartment is greater than 90 percent, the amounts of o- and m- dibromobenzene partitioning into this compartment are not greater than 90 percent. Monobromobenzene and p-dibromobenzene are important for the air compartment according to the Neely's decision tree as their amounts are greater than 90 percent. It is possible to say according to the Neely's decision tree that o- and m- dibromobenzenes are not important for the air compartment,

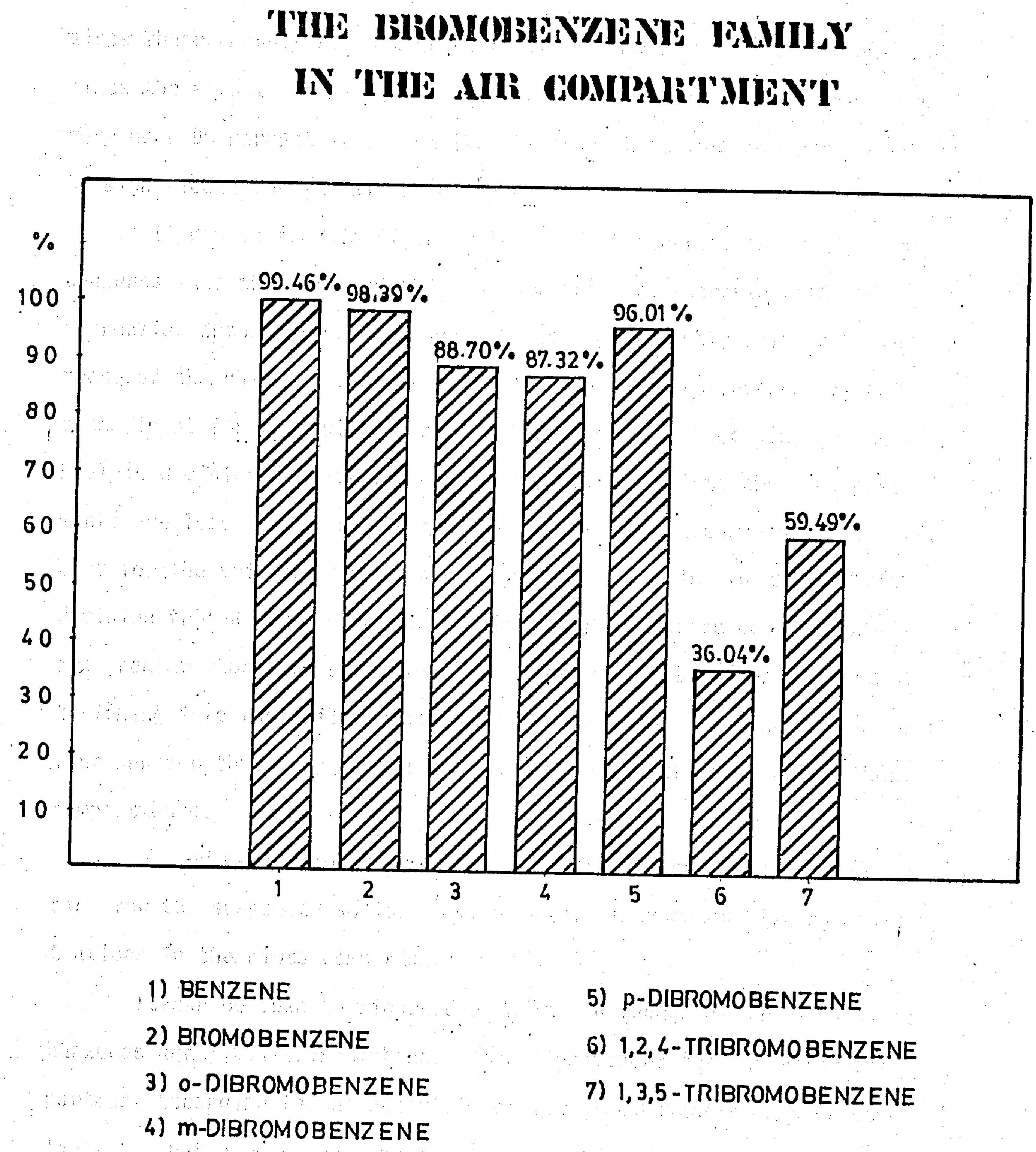


FIGURE 5.3.11. The bargraph of bromobenzene family in the air compartment

since their amounts are not greater than 90 percent. On the other hand since the amounts of o- and m- dibromobenzenes in that compartment are very near 90 percent it can be thought that these two compounds might be significant for the air compartment.

It can be seen in Figure 5.3.12 that the partitioning of bromobenzenes into the soil and sediment compartments increase with the increasing number of bromine substitutes significantly compared with those of the chlorine substitutes. Although p-dibromobenzene is not significant for the soil and sediment compartments according to the Neely's decision tree as its amounts partitioning into these compartments are less than four percent, o- and m- dibromobenzenes are significant for the soil and sediment compartments according to the Neely's decision tree as their amounts partitioning into these compartments are greater than four percent. The amounts of tribromobenzenes partitioning into the soil and sediment compartments are much greater than four percent thus they become very important for the soil and sediment compartments.

o- and m-dibromobenzenes and tribromobenzenes are also significant for the suspended solids compartments. They reach high concentrations in the biota compartment.

It can be seen in Figure 5.3.12 that although o- and m- dibromobenzenes and 1,2,4-tribromobenzene are significant for the water compartment according to the Neely's decision tree as their mass percentages in that compartment are greater than two percent, p-dibromobenzene is not significant for that compartment since its mass percentage in

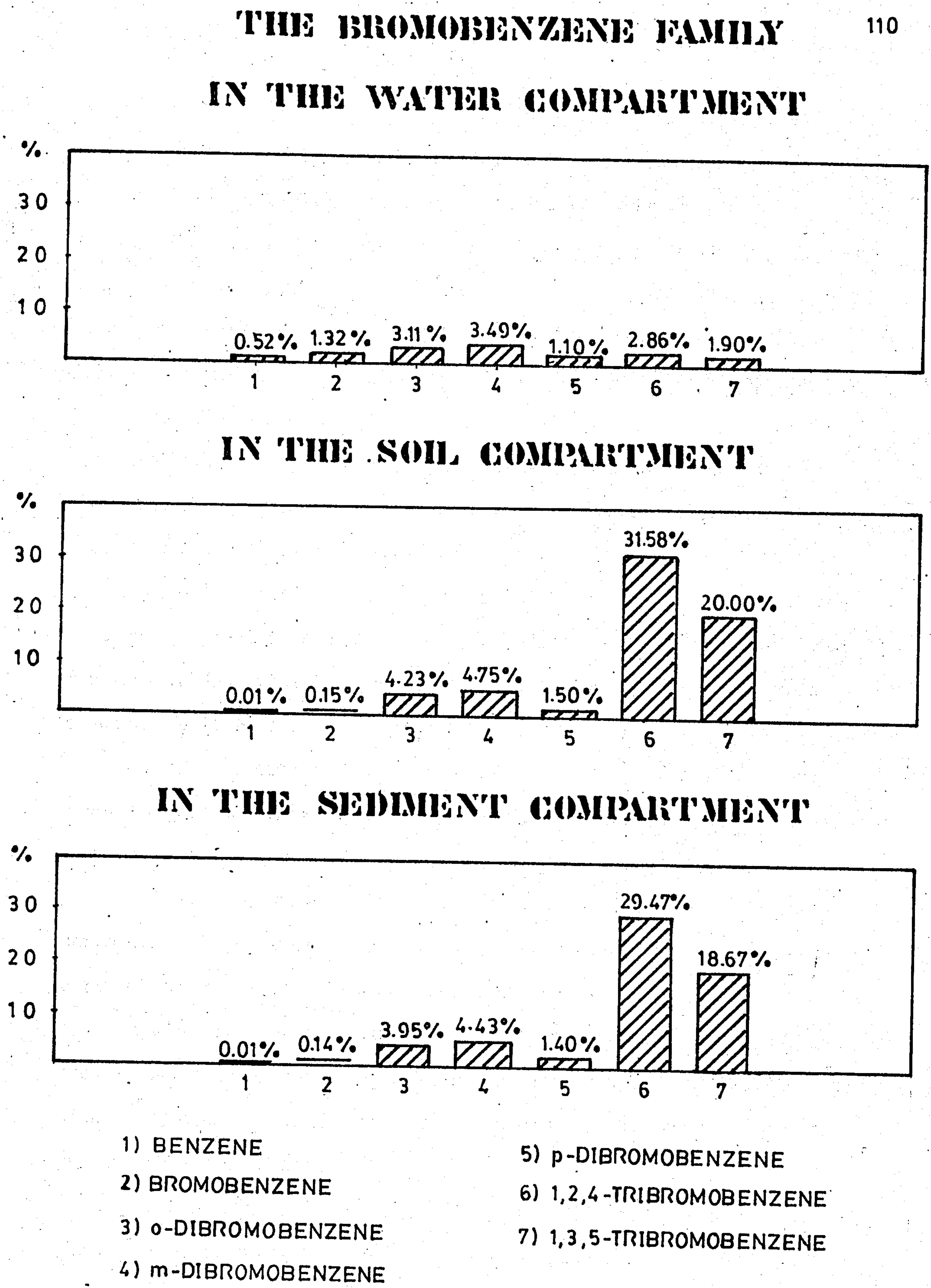


FIGURE 5.3.12. The bargraphs of bromobenzene family in the water, soil and sediment compartments

that compartment is less than two percent. It is possible to say according to the Neely's decision tree that 1,3,5-tribromobenzene is insignificant for the water compartment since its amount partitioning into this compartment is less than two percent. On the other hand, since this amount is very near two percent it can be thought that 1,3,5-tribromobenzene might be significant for the water compartment.

As illustrated in Figure 5.3.13, with the increasing number of iodine substituents, the amount partitioning into the air compartment decreases significantly compared with the bromine substituents. Although monoiodobenzene is significant for the air compartment according to the Neely's decision tree as its amount partitioning into that compartment is greater than 90 percent, diiodobenzenes are not significant for the air compartment since their amounts partitioning into that compartment is less than 90 percent.

It can be seen in Figure 5.3.14 that diiodobenzenes are very important for the soil and sediment compartments as their mass percentages in those compartments are much greater than four percent.

Diiodobenzenes are also important for the suspended solid compartments and they reach the highest concentrations in the biota compartment among the other substituted benzenes.

As can be seen in Figure 5.3.14, monoiodobenzene and diiodobenzenes are significant for the water compartment according to the Neely's decision tree, since their amounts partitioning into that compartment are greater than two percent.

If the benzene is substituted for two different halogen atoms the amount that partition into the air compartment is less than that of

THE IODOBENZENE FAMILY IN THE AIR COMPARTMENT

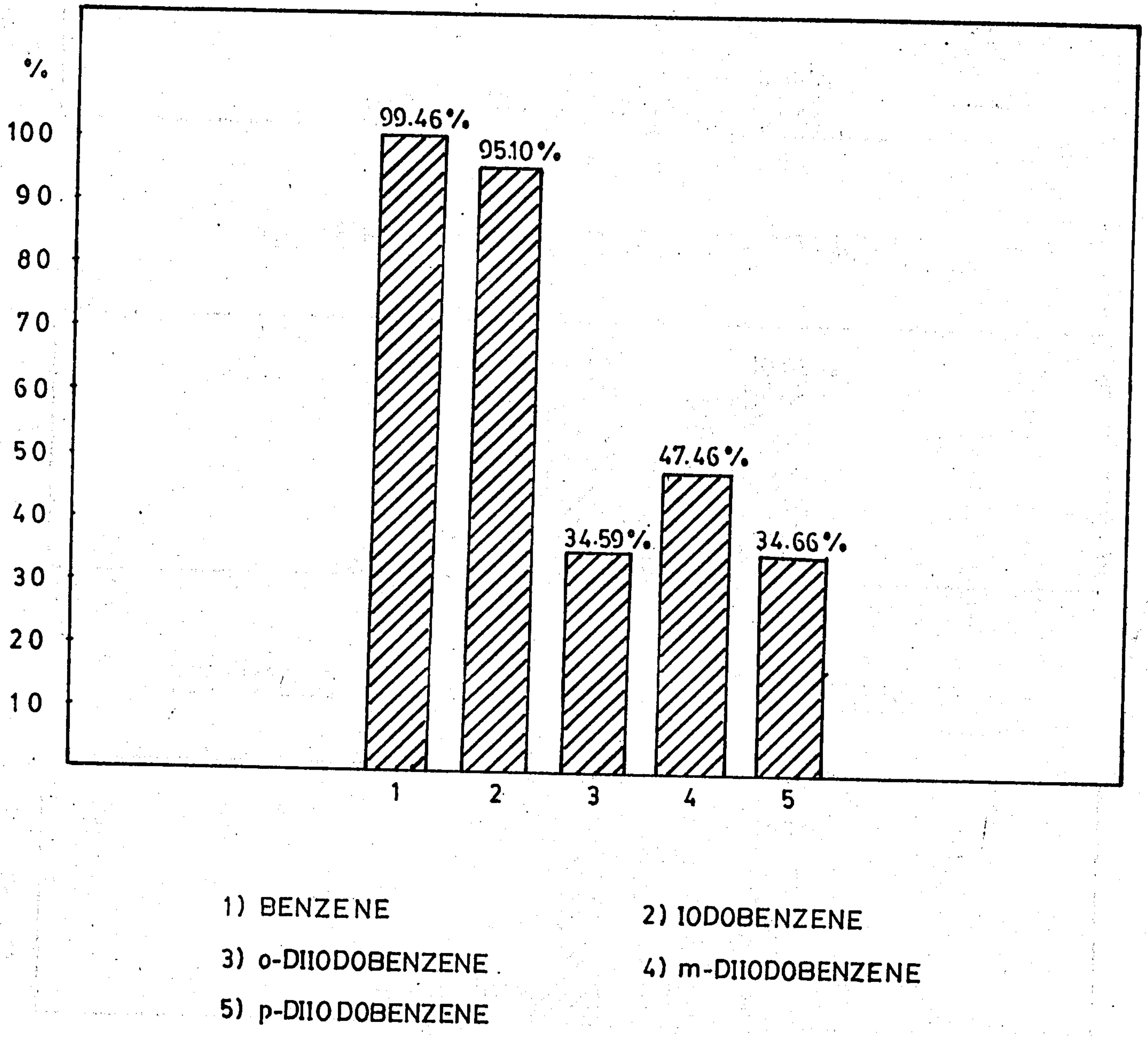


FIGURE 5.3.13. The bargraph of the iodobenzene family in the air compartment

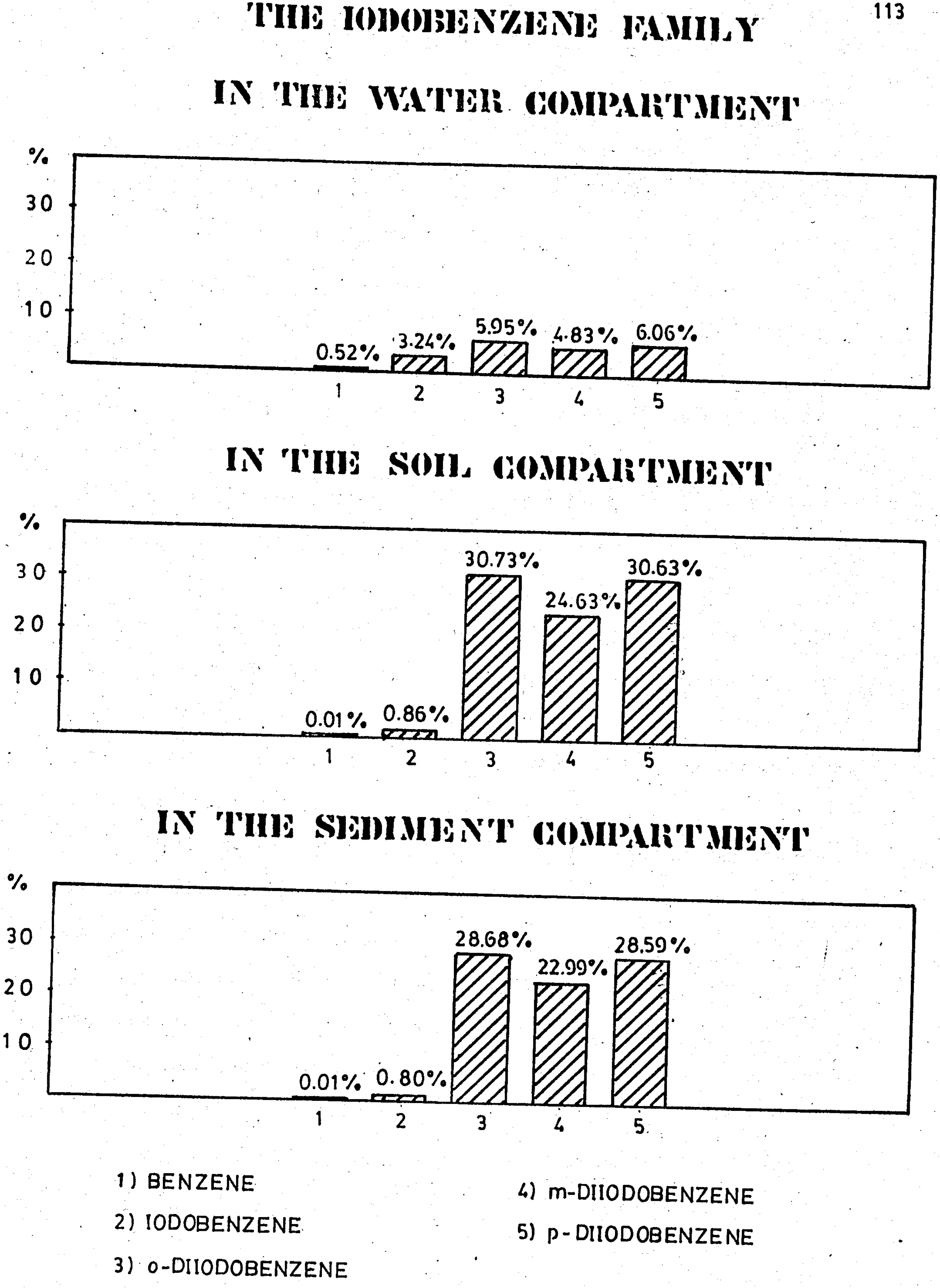


FIGURE 5.3.14. The bargraphs of iodobenzene family in the water, soil and sediment compartments

benzene as illustrated in Figure 5.3.15. The presence of chlorine and bromine together on the benzene ring does not decrease the amount partitioning into the air compartment below the 90 percent and therefore bromochlorobenzenes are significant for the air compartment according to the Neely's decision tree. The presence of chlorine and iodone together on the benzene ring decrease the amount that partitions into the air compartment below the 90 percent and thus it is possible to say according to Neely's decision tree that chloroiodobenzenes are in significant for the air compartment. On the other hand, it can be thought that they might be significant for that compartment since their amounts partitioning into the air compartment are near 90 percent. The presence of iodine and bromine together on the benzene ring decrease the amount of partitioning into the air compartment significantly compared with the others. The bromoiodobenzenes are not significant for the air compartment according to the Neely's decision tree as its amount in the air compartment is less than 90 percent.

It can be seen in Figure 5.3.16 that chloroiodobenzenes and p-bromoiodobenzene significantly partition into the soil and sediment compartments. Their mass percentages in these compartments are greater than four percent. They are also important for the suspended solids compartment.

Chloroiodobenzenes and p-bromoiodobenzene reach high concentrations in the biota compartment.

As can be seen in Figure 5.3.16, chloroiodobenzenes and p-bromoiodobenzene are also significant for the water compartment according to

THE BENZENE FAMILY SUBSTITUTED FOR TWO DIFFERENT HALOGEN IN THE AIR COMPARTMENT

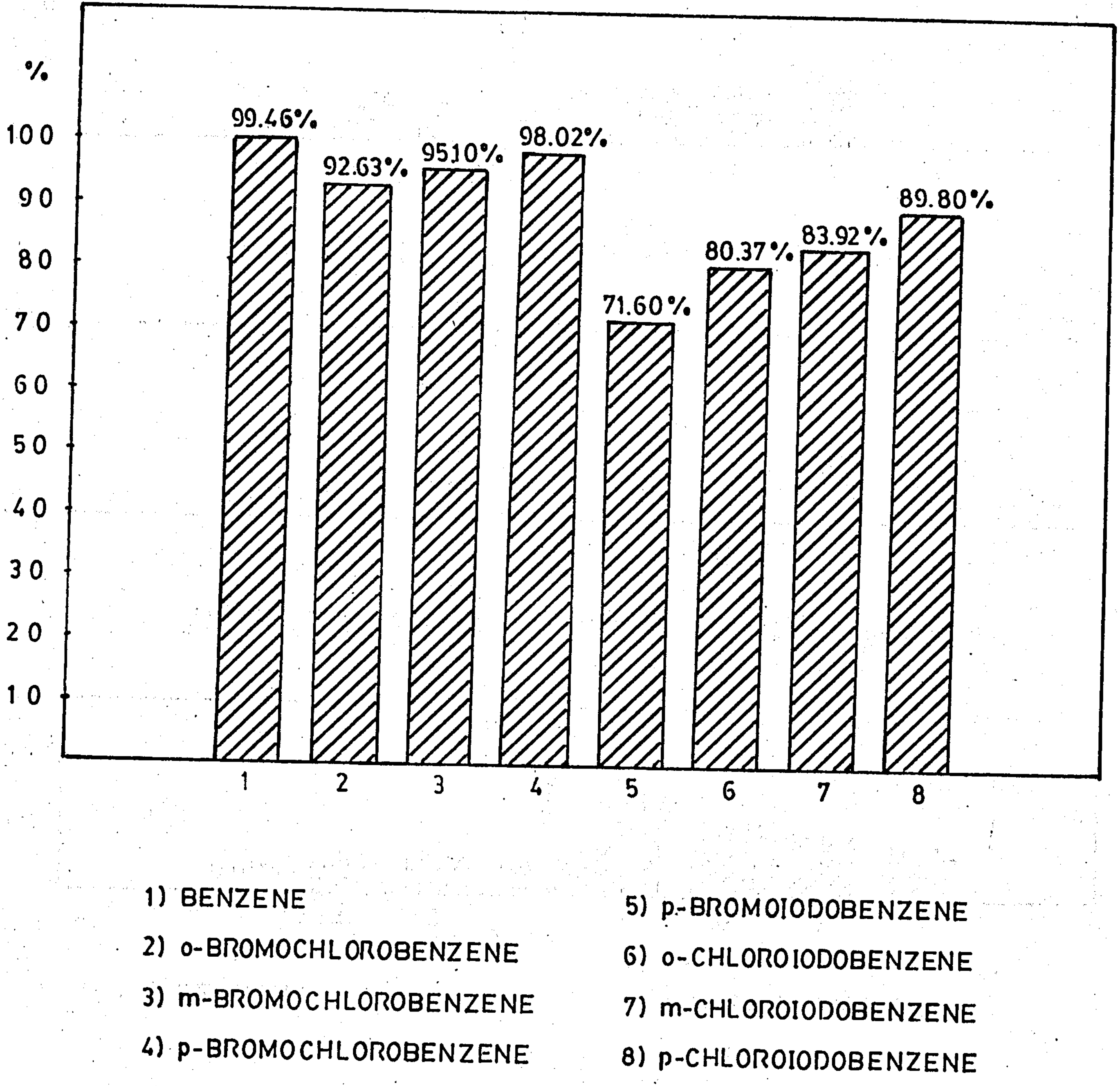
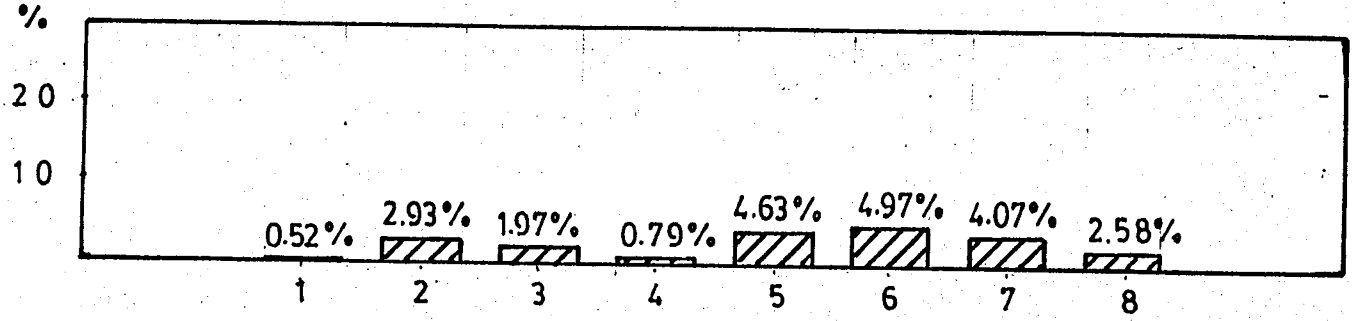


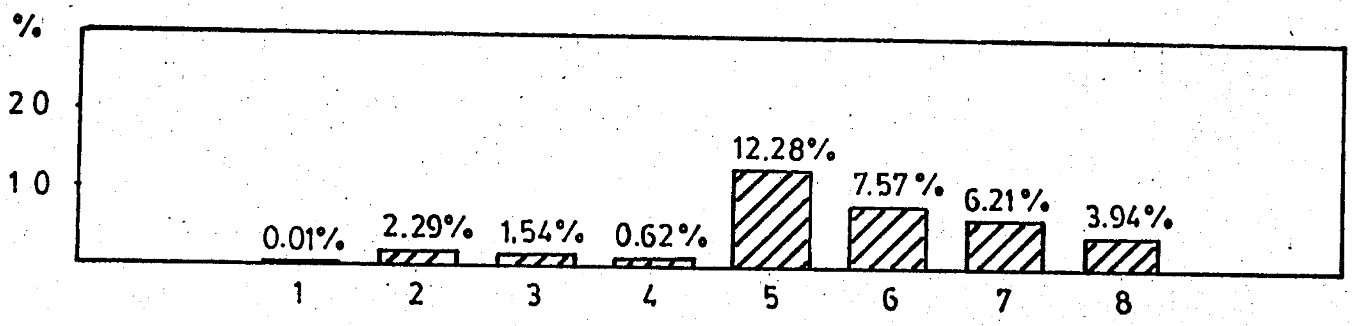
FIGURE 5.3.15. The bargraph of benzene family substituted for two different halogen in the air compartment

THE BENZENE FAMILY SUBSTITUTED FOR TWO DIFFERENT HALOGEN

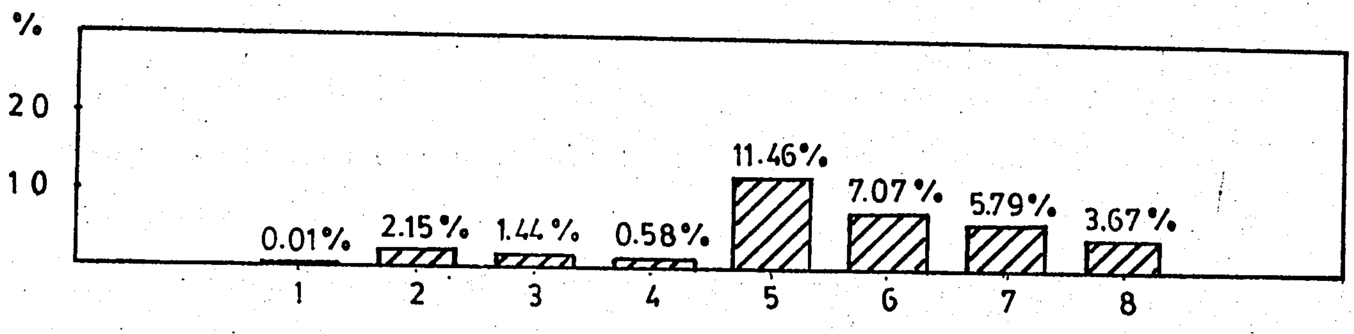
IN THE WATER COMPARTMENT



IN THE SOIL COMPARTMENT



IN THE SEDIMENT COMPARTMENT



1) BENZENE
2) o-BROMOCHLOROBENZENE
3) m-BROMOCHLOROBENZENE
4) p-BROMOCHLOROBENZENE
5) p-BROMOIODOBENZENE
6) o-CHLOROIODOBENZENE
7) m-CHLOROIODOBENZENE
8) p-CHLOROIODOBENZENE

FIGURE 5.3.16. The bargraphs of benzene family substituted for two different halogen in the water, soil and sediment compartments

the Neely's decision tree since their amounts partitioning into that compartment is greater than two percent. Although o-bromochlorobenzene is significant for the water compartment as its amount that partitions into this compartment is greater than two percent, p-bromochlorobenzene is not significant for the water compartment as its mass percentage in that compartment is less than two percent. It is possible to say that according to Neely's decision tree, m-bromochlorobenzene is not significant for the water compartment as its amount in that compartment is less than two percent. On the other hand, it can be thought that this compound might be significant for the water compartment as its amount in that compartment is very near two percent.

Toluene and xylenes are significant for the air compartment according to Neely's decision tree as their mass percentages in that compartment are greater than 90 percent as illustrated in Figure 5.3.17. The amounts of xylenes partitioning into the air compartment decrease slightly compared with that of toluene. Nitrotoluenes partition into the air compartment in the lesser amounts than toluene and xylenes. They are not significant for the air compartment according to the Neely's decision tree since their mass percentages are not greater than 90 percent.

It can be seen in Figure 5.3.18 that toluenes substituted for a polar group such as hydroxyl or amino group mostly partitions into the water compartment. Since their amounts partitioning into that compartment are much greater than two percent, according to the Neely's decision tree they become significant for the water compartment. Nitrotoluenes partition into the water compartment in the lesser amounts

THE TOLUENE FAMILY IN THE AIR COMPARTMENT

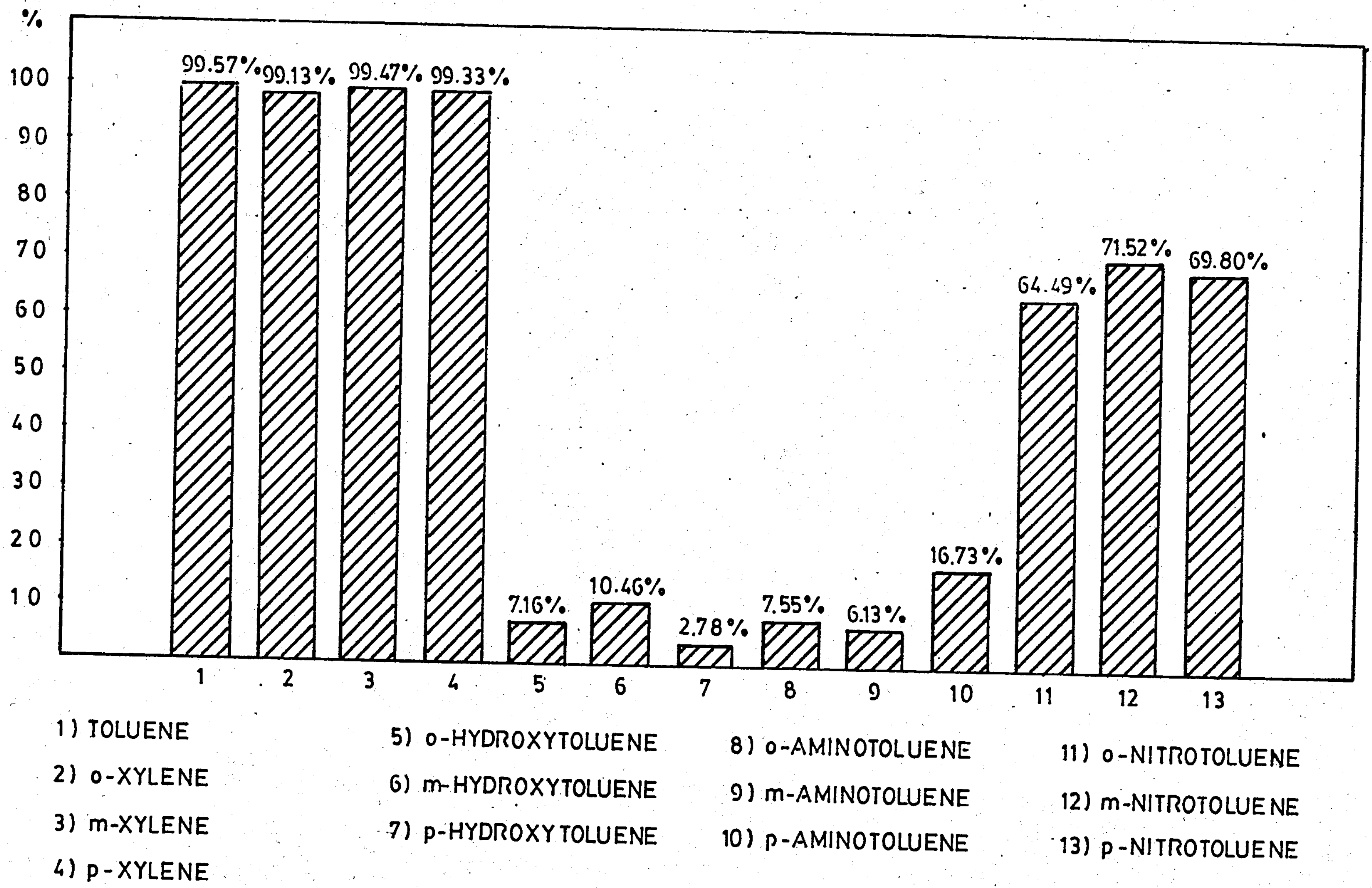


FIGURE 5.3.17 The bargraph of toluene family in the air compartment

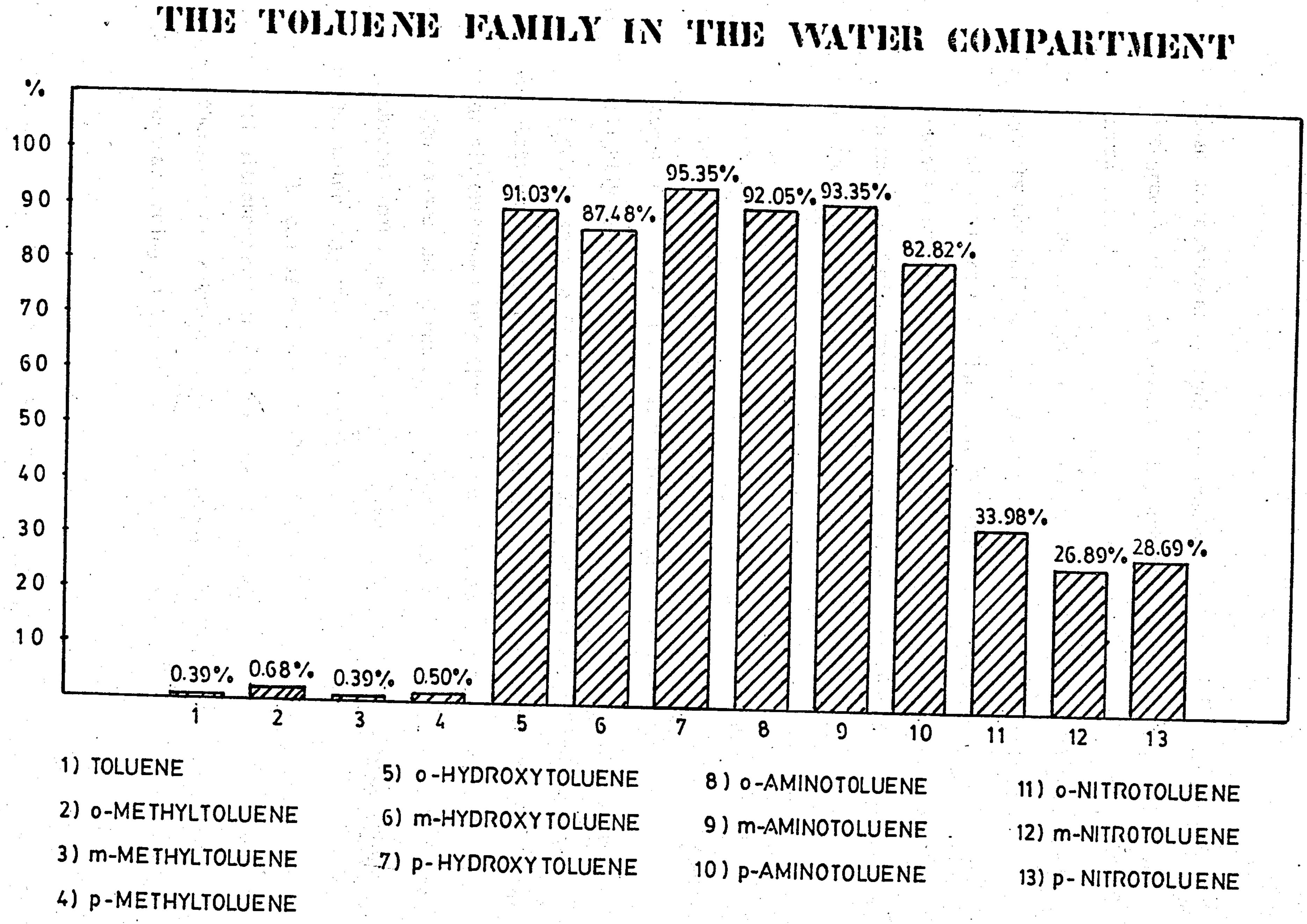


FIGURE 5.3.18. The bargraph of toluene family in the water compartment

than aminotoluenes or hydroxytoluenes since their mass percentages are greater than two percent they are also significant for the water compartment.

It can be seen in Figure 5.3.19 and Figure 5.3.20 that all phenols and anilines mostly partition into the water compartment. All of them are very important for the water compartment, since their amounts partitioning into this compartment are much greater than two percent. For dihydroxy benzenes and diaminobenzenes mass percentages in the water compartment are greater than 99.5 percent.

Nitrobenzenes partition either into the air compartment or into the water compartment. While 41.95 percent of nitrobenzene partitions into the air compartment, 57.14 percent of it partitions into the water compartment. The amount partitioning into the water compartment is slightly greater than the amount partitioning into the air compartment. It can be seen in Figure 5.3.21 and Figure 5.3.22 that the second substituted group on the benzene ring greatly influence the partitioning of nitrobenzenes into these two compartments. Methyl group substitution causes the amount partitioning into the air compartment to increase whereas amino and hydroxyl groups cause the amount partitioning into the water compartment to increase.

It can be seen in Figure 5.3.21 that the mass percentages of all nitrobenzenes in the air compartment are less than 90 percent therefore all nitrobenzenes are not significant for the air compartment according to the Neely's decision tree.

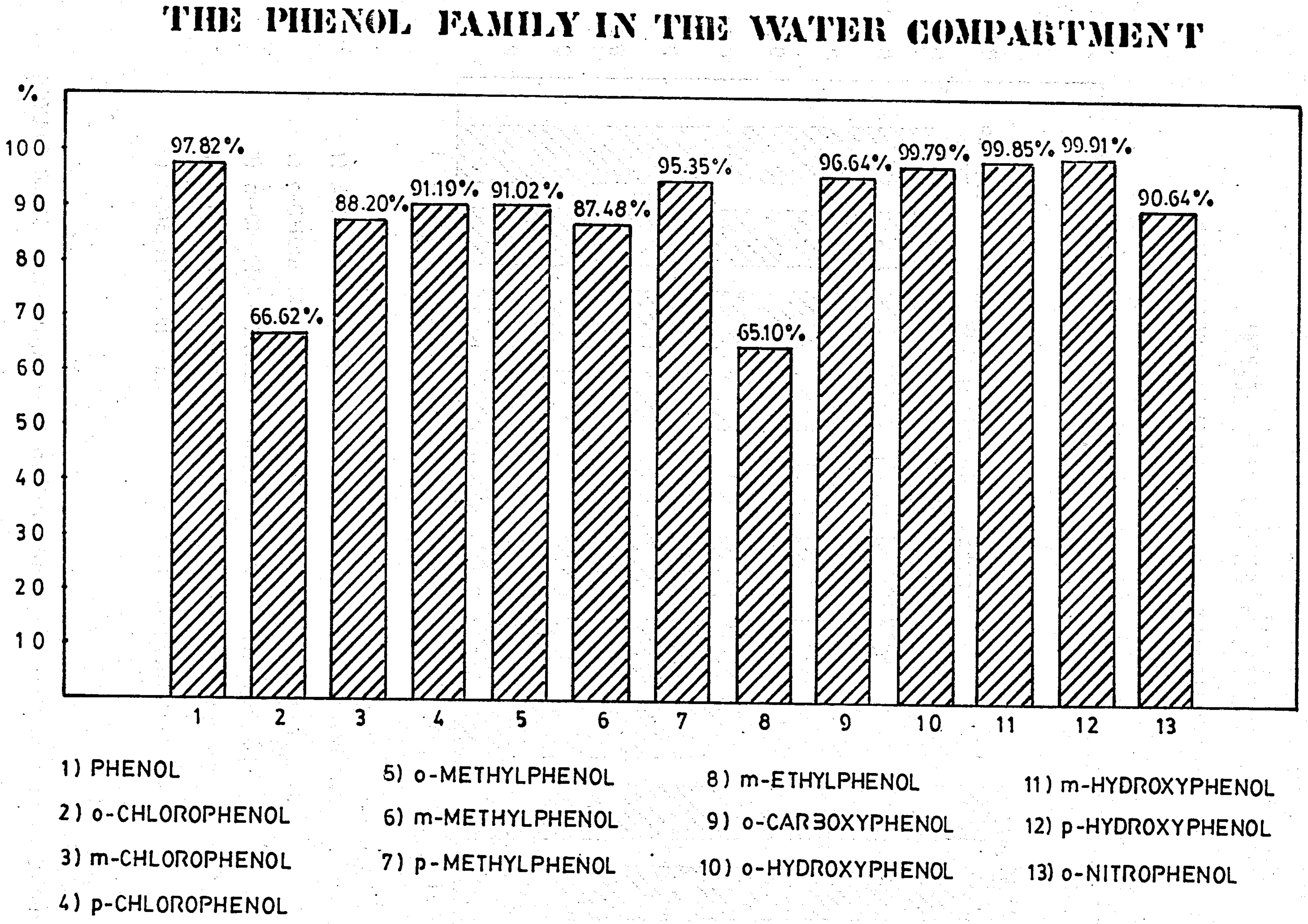
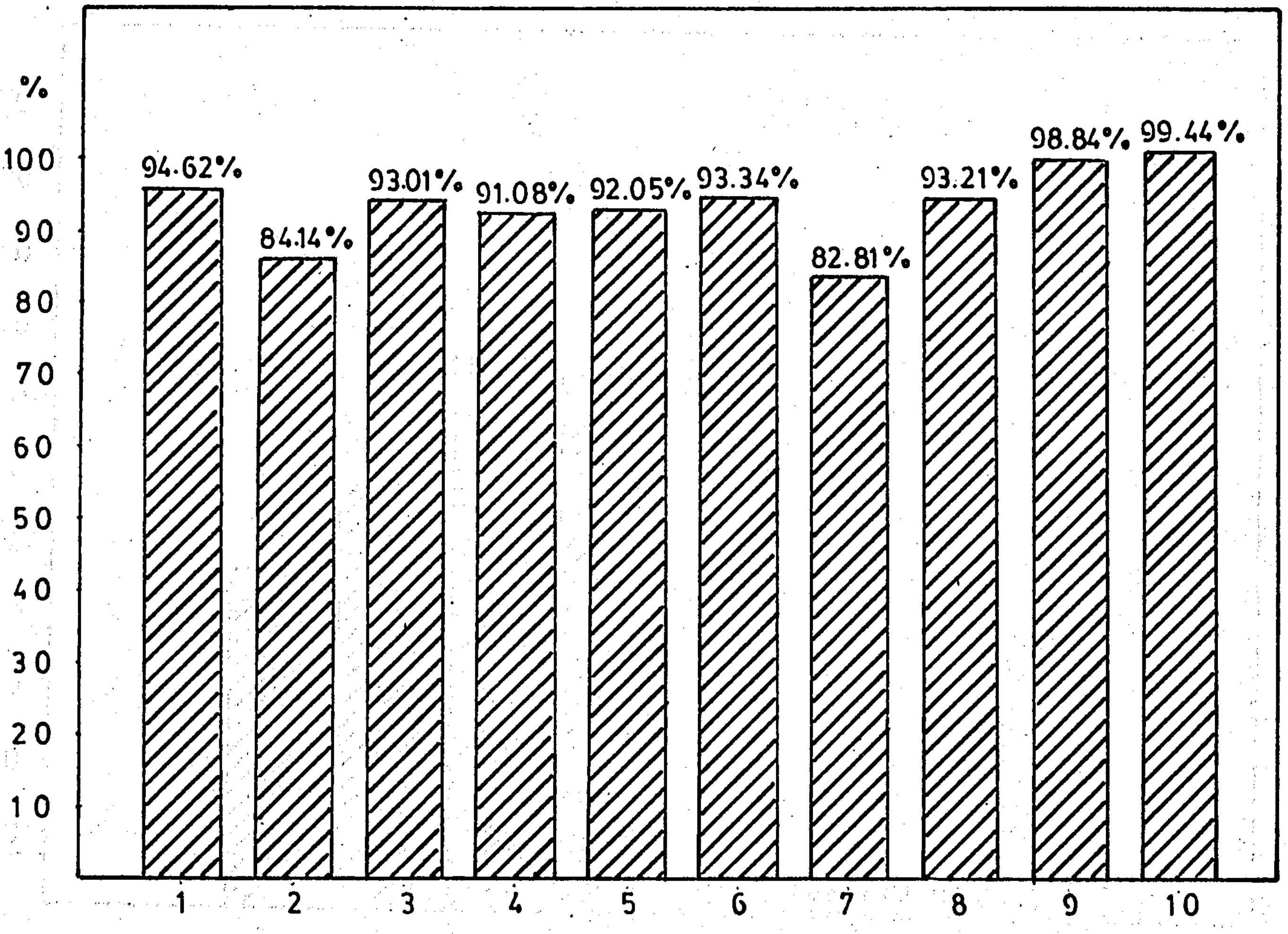


FIGURE 5.3.19. The bargraph of phenol family in the water compartment

THE ANILINE FAMILY IN THE WATER COMPARTMENT



1) ANILINE
2) o-CHLOROANILINE
3) m-CHLOROANILINE
4) p-CHLOROANILINE
5) o-METHYLANILINE
6) m-METHYLANILINE
7) p-METHYLANILINE
8) o-NITROANILINE
9) m-NITROANILINE
10) p-NITROANILINE

FIGURE 5.3.20. The bargraph of aniline family in the water compartment

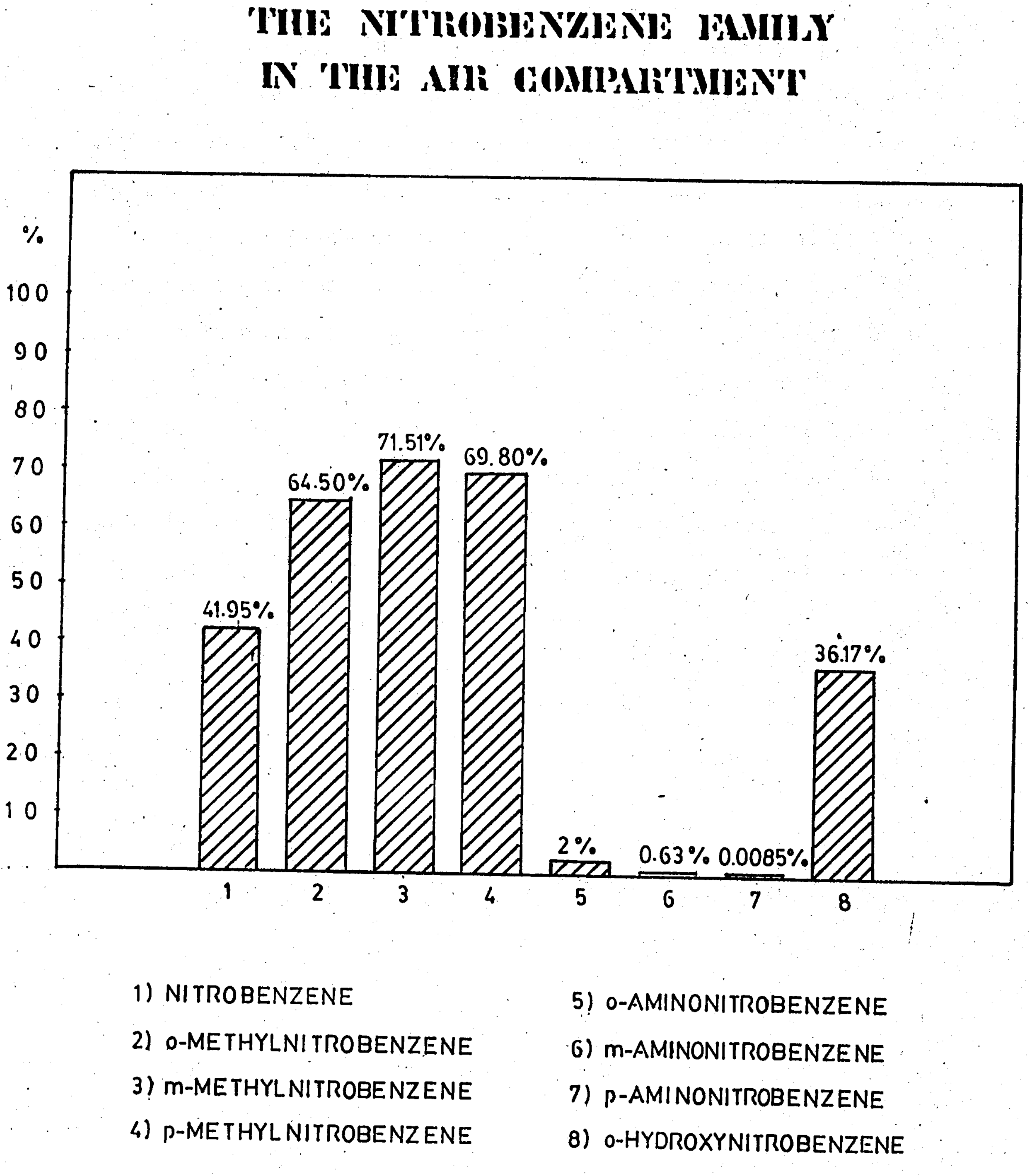
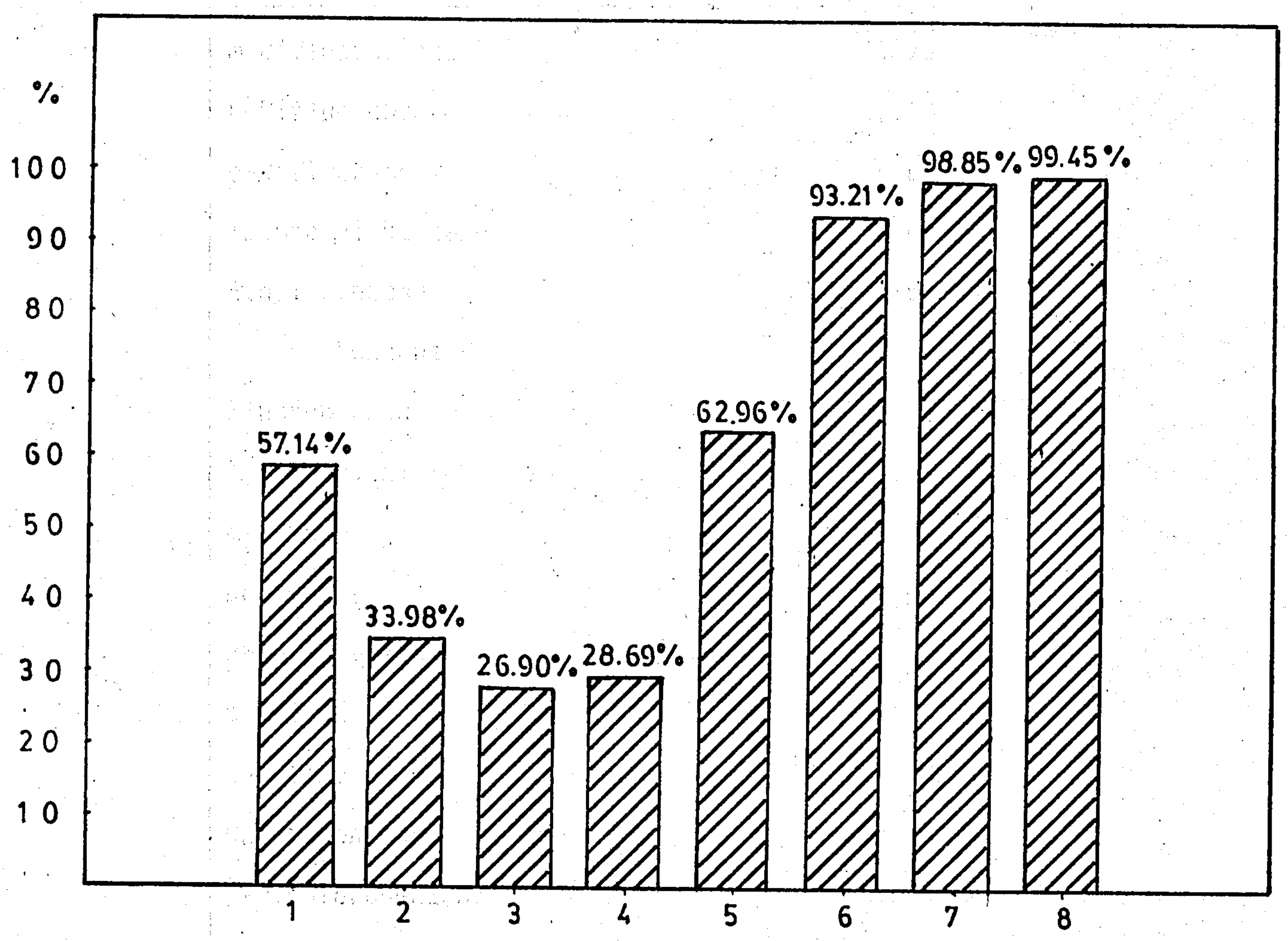


FIGURE 5.3.21. The bargraph of nitrobenzene family in the air compartment

It can be seen in Figure 5.3.22 that the mass percentages of all nitrobenzenes in the water compartment are greater than two percent therefore all nitrobenzenes are significant for the water compartment according to the Neely's decision tree.

Analysis of the resulting pattern thus indicates the compartment offering the best chance for maximum degradation. The results arranged to rank the substituted benzenes by their potentials to contaminate each compartment is given in Table 5.3.1, Table 5.3.2, Table 5.3.3, Table 5.3.4, Table 5.3.5 and Table 5.3.6. The advantage of this ranking is that it makes the chemicals with the greatest potential to contaminate each compartment quite obvious. The next step would be to examine these chemicals critically in order to see if they truly are a problem or not.

THE NITROBENZENE FAMILY IN THE WATER COMPARTMENT



1) NITROBENZENE
2) o-METHYLNITROBENZENE
3) m-METHYLNITROBENZENE
4) p-METHYLNITROBENZENE
5) o-HYDROXYNITROBENZENE
6) o-AMINONITROBENZENE
7) m-AMINONITROBENZENE
8) p-AMINONITROBENZENE

FIGURE 5.3.22. The bargraph of nitrobenzene family in the water compartment

TABLE 5.3.1 - Ranking of Substituted Benzenes by Their Potentials to Contaminate the Air Compartment

CHEMICAL	% IN AIR
m-Difluorobenzene	99.73
p-Difluorobenzene	99.64
o-Difluorobenzene	99.62
Isopropyl benzene	99.60
Ethyl benzene	99.58
Methyl benzene	99.57
Fluorobenzene	99.53
1,3,5-Trichlorobenzene	99.52
m-Xylene	93.47
Benzene	99.46
Propyl benzene	99.40
p-Xylene	99.33
o-Xylene	99.13
Chlorobenzene	99.09
p-Dichlorobenzene	99.08
m-Dichlorobenzene	98.54
Bromobenzene	98.39
p-Bromochlorobenzene	98.02
o-Dichlorobenzene	97.11
1,2,4-Trichlorobenzene	96.47
p-Dibromobenzene	96.01
1,2,3-Trichlorobenzene	95.31

Table 5.3.1 - Continued...

CHEMICAL	% IN AIR
Iodobenzene	95.09
m-Bromochlorobenzene	95.06
Pentachlorobenzene	93.34
1,2,4,5-Tetrachlorobenzene	93.05
1,2,3,5-Tetrachlorobenzene	92.98
o-Bromochlorobenzene	92.63
p-Chloroiodobenzene	89.80
o-Dibromobenzene	88.69
m-Dibromobenzene	87.32
1,2,3,4-Tetrachlorobenzene	84.14

TABLE 5.3.2 - Ranking of Substituted Benzenes by Their Potentials to Contaminate the Soil Compartment

CHEMICAL	% IN SOIL
1,2,4-Tribromobenzene	31.58
o-Diiodobenzene	30.73
p-Diiodobenzene	30.63
m-Diiodobenzene	24.63
Hexachlorobenzene	20.85
1,3,5-Tribromobenzene	20.00
p-Bromoiodobenzene	12.28
1,2,3,4-Tetrachlorobenzene	7.88
o-Chloroiodobenzene	7.57
m-Chloroiodobenzene	6.21
m-Dibromobenzene	4.75
o-Dibromobenzene	4.23
p-Chloroiodobenzene	3.94
1,2,3,5-Tetrachlorobenzene	3.49
Pentachlorobenzene	3.34
1,2,4,5-Tetrachlorobenzene	3.28

TABLE 5.3.3 - Ranking of Substituted Benzenes by Their Potential to Contaminate the Water Compartment

CHEMICAL	% IN WATER
p-Hydroxylphenol	99.91
m-Phenylenediamine	99.87
m-Hydroxyphenol	99.86
o-Hydroxyphenol	99.79
p-Nitroaniline	99.44
Benzyl alcohol	99.01
m-Nitroaniline	98.85
Phenol	98.02
p-Methylphenol	95.35
p-Chloroaniline	95.00
Aniline	94.63
m-Methylaniline	93.35
o-Nitroaniline	93.21
m-Chloroaniline	93.01
o-Methylaniline	92.05
p-Chlorophenol	91.19
o-Methylphenol	91.02
o-Nitrophenol	90.65
Acetophenone	89.44
m-Chlorophenol	88.20
m-Methylphenol	87.48
o-Chloroaniline	84.14

TABLE 5.3.3 - Continued..

CHEMICAL	% IN WATER
p-Methylaniline	82.81
o-Chlorophenol	66.62
m-Ethylphenol	65.10
o-Hydroxynitrobenzene	62.96
Nitrobenzene	57.14
Butylbenzene	41.99
Anisole	37.79
o-Methylnitrobenzene	33.98
p-Methylnitrobenzene	28.69
m-Methylnitrobenzene	26.90
N,N-Dimethylaniline	22.98
p-Diiodobenzene	6.06
o-Diiodobenzene	5.94
o-Chloroiodobenzene	4.97
p-Bromoiodobenzene	4.63
m-Diiodobenzene	4.88
m-Chloroiodobenzene	4.07
m-Dibromobenzene	3.49
Iodobenzene	3.24
o-Dibromobenzene	3.11
o-Bromochlorobenzene	2.93
1,2,4-Tribromobenzene	2.86
p-Chloroiodobenzene	2.58
m-Bromochlorobenzene	1.97
1,3,5-Tribromobenzene	1.81

TABLE 5.3.4 - Ranking of Substituted Benzenes by Their Potential Concentrations in the Biota Compartment

CHEMICAL	C_{biota} (ppm)
p-Diiodobenzene	5.012 E-1
o-Diiodobenzene	5.011 E-1
1,2,4-Tribromobenzene	4.385 E-1
m-Diiodobenzene	4.033 E-1
1,3,5-Tribromobenzene	2.777 E-1
Hexachlorobenzene	2.403 E-1
p-Bromoiodobenzene	1.898 E-1
o-Chloroiodobenzene	1.070 E-1
m-Chloroiodobenzene	8.780 E-2
1,2,3,4-Tetrachlorobenzene	7.327 E-2
m-Dibromobenzene	6.764 E-2
o-Dibromobenzene	6.030 E-2
p-Chloroiodobenzene	5.570 E-2
m-Chlorophenol	4.310 E-2
o-Nitroaniline	3.720 E-2
p-Chlorophenol	3.593 E-2
1,2,4,5-Tetrachlorobenzene	3.470 E-2
Pentachlorobenzene	3.437 E-2
1,2,3,5-Tetrachlorobenzene	3.244 E-2
o-Bromochlorobenzene	2.880 E-2
m-Ethylphenol	2.486 E-2
p-Dibromobenzene	2.129 E-2
1,2,3-Trichlorobenzene	1.998 E-2

TABLE 5.3.4 - Continued..

CHEMICAL	C_{biota} (ppm)
m-Bromochlorobenzene	1.930 E-2
o-Chlorophenol	1.640 E-2
1,2,4-Trichlorobenzene	1.486 E-2
m-Methyl phenol	1.405 E-2
Iodobenzene	1.350 E-2
m-Chloroaniline	1.340 E-2
p-Methyl phenol	1.309 E-2
o-Methyl phenol	1.275 E-2
o-Chloroaniline	1.261 E-2
p-Chloroaniline	1.242 E-2
m-Methylnitrobenzene	1.198 E-2
o-Methylnitrobenzene	1.197 E-2
o-Nitrophenol	1.190 E-2
p-Methylnitrobenzene	1.159 E-2
p-Bromochlorobenzene	7.730 E-3
Nitrobenzene	7.493 E-3
N,N-Dimethylaniline	7.297 E-3
o-Dichlorobenzene	7.280 E-3
Anisole	7.240 E-3
Butylbenzene	7.117 E-3
Acetophenone	6.748 E-3
p-Nitroaniline	5.947 E-3
m-Nitroaniline	5.684 E-3

TABLE 5.3.4 - Continued..

CHEMICAL	C_{biota} (ppm)
Phenol	4.575 E-3
m-Methylaniline	4.416 E-3
p-Methylaniline	3.842 E-3
m-Dichloroaniline	3.670 E-3
o-Methylaniline	3.511 E-3
Benzyl alcohol	2.628 E-3
1,3,5-Trichlorobenzene	2.064 E-3
Bromobenzene	2.050 E-3
p-Dichlorobenzene	1.870 E-3
o-Hydroxyphenol	1.753 E-3
m-Hydroxyphenol	1.500 E-3
Aniline	1.462 E-3
Propyl benzene	1.322 E-3
m-Phenylenediamine	1.300 E-3
p-Hydroxyphenol	9.951 E-4
o-Xylene	9.283 E-4
Isopropylbenzene	8.638 E-4
p-Xylene	7.597 E-4
Chlorobenzene	6.540 E-4
m-Xylene	6.239 E-4
Ethylbenzene	4.636 E-4
Methyl benzene	1.970 E-4
o-Difluorobenzene	1.784 E-4

TABLE 5.3.4 - Continued..

CHEMICAL	C_{biota} (ppm)
p-Difluorobenzene	1.665 E-4
m-Difluorobenzene	1.223 E-4
Fluorobenzene	1.043 E-4
Benzene	7.480 E-5

TABLE 5.3.5 - Ranking of Substituted Benzenes by Their Potential Concentrations in the Suspended Solids Compartment.

CHEMICAL	$C_{\text{suspended solids}}$ (ppm)
o-Diiodobenzene	3.004 E-1
p-Diiodobenzene	2.994 E-1
1,2,4-Tribromobenzene	2.945 E-1
m-Diiodobenzene	2.467 E-1
1,3,5-Tribromobenzene	1.866 E-1
Hexachlorobenzene	1.760 E-1
p-Bromoiodobenzene	1.029 E-1
o-Chloroiodobenzene	5.352 E-2
1,2,3,4-Tetrachlorobenzene	5.042 E-2
m-Chloroiodobenzene	4.386 E-2
m-Dibromobenzene	3.318 E-2
o-Dibromobenzene	2.959 E-2
p-Chloroiodobenzene	2.781 E-2
Pentachlorobenzene	2.481 E-2
1,2,3,5-Tetrachlorobenzene	2.232 E-2
1,2,4,5-Tetrachlorobenzene	2.097 E-2
o-Bromochlorobenzene	1.300 E-2
m-Chlorophenol	1.229 E-2
1,2,3-Trichlorobenzene	1.050 E-2
p-Dibromobenzene	1.045 E-2
o-Nitroaniline	1.011 E-2
p-Chlorophenol	9.867 E-3
m-Bromochlorobenzene	8.723 E-3
1,2,4-Trichlorobenzene	7.563 E-3

TABLE 5.3.5 - Continued....

CHEMICAL	$C_{\text{suspended solids}}$ (ppm)
m-Ethylphenol	6.850 E-3
Iodobenzene	5.194 E-3
o-Chlorophenol	4.148 E-3
m-Methylphenol	3.396 E-3
p-Bromochlorobenzene	3.492 E-3
m-Methylnitrobenzene	3.327 E-3
o-Methylnitrobenzene	3.188 E-3
p-Methylnitrobenzene	3.163 E-3
m-Chloroaniline	3.086 E-3
p-Methylphenol	3.079 E-3
o-Dichlorobenzene	3.026 E-3
o-Methylphenol	3.008 E-3
o-Chloroaniline	2.924 E-3
p-Chloroaniline	2.810 E-3
o-Nitrophenol	2.666 E-3
N,N-Dimethylaniline	1.949 E-3
o-Hydroxynitrobenzene	1.852 E-3
Anisole	1.805 E-3
Nitrobenzene	1.708 E-3
Butylbenzene	1.671 E-3
m-Dichlorobenzene	1.525 E-3
Acetophenone	1.401 E-3
p-Nitroaniline	1.156 E-3
m-Nitroaniline	1.097 E-3
1,3,5-Trichlorobenzene	1.085 E-3

TABLE 5.3.5 - Continued...

CHEMICAL	$C_{suspended\ solids}$ (ppm)
Phenol	9.122 E-4
m-Methylaniline	8.615 E-4
Propylbenzene	8.508 E-4
p-Methylaniline	7.468 E-4
p-Dichlorobenzene	7.246 E-4
Bromobenzene	6.940 E-4
o-Methylaniline	6.594 E-4
Benzyl Alcohol	4.622 E-4
Isopropylbenzene	3.678 E-4
o-Xylene	3.280 E-4
o-Hydroxyphenol	2.858 E-4
p-Xylene	2.741 E-4
Aniline	2.400 E-4
m-Hydroxyphenol	2.379 E-4
m-Xylene	2.267 E-4
Chlorobenzene	2.098 E-4
m-Phenylenediamine	2.016 E-4
Ethyl benzene	1.655 E-4
p-Hydroxyphenol	1.468 E-4
Methylbenzene	6.008 E-5
o-Difluorobenzene	5.251 E-5
p-Difluorobenzene	4.882 E-5
m-Difluorobenzene	3.586 E-5
Fluorobenzene	2.747 E-5
Benzene	1.878 E-5

TABLE 5.3.6 - Ranking of Substituted Benzenes by Their Potentials to Contaminate the Sediment Compartment

CHEMICAL	% IN SEDIMENT
1,2,4-Tribromobenzene	29.47
o-Diiodobenzene	28.68
m-Diiodobenzene	22.59
p-Diiodobenzene	28.59
1,3,5-Tribromobenzene	18.67
Hexachlorobenzene	16.47
p-Bromoiodobenzene	11.46
1,2,3,4-Tetrachlorobenzene	7.36
o-Chloroiodobenzene	7.07
m-Chloroiodobenzene	5.79
m-Dibromobenzene	4.43
o-Dibromobenzene	3.95
p-Chloroiodobenzene	3.67
Pentachlorobenzene	3.12
1,2,3,5-Tetrachlorobenzene	3.26
1,2,4,5-Tetrachlorobenzene	3.06
m-Chlorophenol	3.01

VI. CORRELATIONS

The partitioning behaviour of chemicals entering the environment is governed by their physical and chemical properties such as solubility, vapor pressure, and n-octanol-water partition coefficients. With this in mind, in this thesis, the influence of solubility and vapor pressure on the partitioning behaviour of a chemical having a mean molecular weight of 150 g are investigated through Mackay's Level I Fugacity Model and the results are given in Table 6.1.1. The chemical having a vapor pressure of 10^6 mm Hg partitions ultimately into the air compartment even if it has a solubility of 10^6 ppm. While the vapor pressure of the chemical is decreasing the amount partitioning into the air compartment decreases. When the vapor pressure of the chemical is less than 10^6 mm Hg, the amount partitioning into the water compartment increases with the increasing solubility. When the chemical has a low vapor pressure and low water solubility it becomes an important contaminant for the soil, sediment and biota compartments.

In this thesis, an investigation is made to find if a simple relationship could be established between the other physicochemical properties of a chemical related to solubility and n-octanol-water

a	s	w
b	ss	sd

TABLE 6.1.1 - The Partitioning of a Chemical having a Mean Molecular Weight of 150 g Between the Compartments of Unit World.

S ppm \ P mm Hg	$1x10^{-6}$			$1x10^{-2}$			$1x10^{2}$			$1x10^{6}$		
$1x10^{-6}$	9.519	46.76	0.001	99.91	0.049	0	100	0	0	100	0	0
	0.004	0.070	43.64	0	0	0.046	0	0	0	0	0	0
$1x10^{-2}$	0.497	51.05	0.719	98.04	1.006	0.014	100	0	0	100	0	0
	0.012	0.008	47.64	0	0.02	0.939	0	0	0	0	0	0
$1x10^{2}$	0.005	11.53	77.69	34.96	7.497	50.53	99.98	0.002	0.01	100	0	0
	0.007	0.018	10.76	0.004	0.012	7.000	0	0	0.002	0	0	0
$1x10^{6}$	0	0.031	99.94	0.007	0.031	99.93	40.88	0.018	59.08	100	0	0
	0	0	0.029	0	0	0.029	0	0	0.017	0	0	0

partition coefficient and its partitioning behaviour into the environmental compartments.

One of the physicochemical properties that is related to n-octanol-water partition coefficient is π-substituent constant given by Eq. (2.21).

$$\log K_{ow}(RX) - \log K_{ow}(RH) = \pi(X) \tag{2.21}$$

where $\log K_{ow}(RX)$ is the logarithm of partition coefficient of the chemical in question, $\log K_{ow}(RH)$ is the logarithm of the partition coefficient of the parent structure, π is the substituent constant.

The second property is the total molecular surface area, TSA. Langmuir first introduced the concept that the surface area of the solute is a determinant of its activity. This concept considers that the major factor in solubility relationships is the energy required to create a cavity in the solvent into which the solute is placed. The energy needed for the hole formation was considered to be proportional to the surface area of the solute. Realizing the difficulty and importance of surface area measurements, Hermann [53] has developed a computer program for estimation of surface area of nonspherical molecules with fixed conformation. For the program, the molecule is considered as a collection of intersecting spheres comprised of individual atoms or molecular groups with each radius located at the nuclear center, standard interatomic bond lengths, bond angles, Van der Waals radii and torsional angles between various atoms in a molecule are the required input for the program. A radius for the solvent (water) may be added to each radius on the solute molecule. Planes of intersection between spheres are used to estimate the contribution to surface area from individual atoms or groups. The program computes the surface area of individual atoms or groups by numerical integration, and the overlap due to intersecting spheres is excluded from the calculation. Total molecular surface area is calculated by the summation of individual group contributions.

Solubility of aliphatic alcohols correlated with their total surface areas by Lande and BanerJee [24] and the following equation was obtained

$$\log S = -0.0317(\mathrm{TSA}) + 3.80 \qquad (6.1)$$

S = mole/litre, TSA = A°^{2}, $n = 75$, $r = 0.986$

The correlation equation between solubility of 26 mono and multi-halogenated benzenes and their TSAs was studied by Yalkowsky et al [16] and given by

$$\log S = -0.0103(t_m) - 0.04225(\mathrm{TSA}) + 0.3290 \qquad (6.2)$$

S = mole/litre, t_m = °C, TSA = A°^{2}, $n = 35$, $r = 0.997$

Lande and Banargee [24] studied the relationship between solubility and total molecular surface area for polynuclear aromatic hydrocarbons, and they developed that equation

$$\log S = -0.0339(\mathrm{TSA}) - 2.10 \qquad (6.3)$$

S = mole/litre, TSA = A°^{2}, $n = 6$, $r = 0.984$

Yalkowsky et al [47] studied the correlation between water solubilites of 31 polycyclic aromatic hydrocarbons and indan and their total molecular surface areas, the following relationship was obtained

$$\log S = -0.0282(\text{TSA}) - 0.0095(t_m) + 1.42 \qquad (6.4)$$

S = mole/litre, TSA = $A^{\circ 2}$, t_m = °C, $n = 32$, $r = 0.9877$

Yalkowsky et al [47] correlated n-octanol-water partition coefficient of those compounds with their total molecular surface areas, and the relationship was given by the following equation

$$\log K_{ow} = 0.0303(\text{TSA}) - 1.389 \qquad (6.5)$$

TSA = $A^{\circ 2}$, $n = 32$, $r = 0.987$

The third physicochemical property that related to solubility and n-octanol-water partition coefficient is molar volume, MV, which can be calculated as the ratio of molecular weight and density.

Lande and Banergee [24] correlated solubility of alkanes with their molar volumes and the following equation was obtained

$$\log S = -0.0299(\text{MV}) + 0.103 \qquad (6.6)$$

S = mole/litre, MV = cm^3/mole, $n = 13$, $r = 0.887$

They also developed a correlation between solubility and molar volume for cycloalkenes [24]

$$\log S = -0.0362(\text{MV}) + 1.21 \qquad (6.7)$$

S = mole/litre, MV = cm^3/mole, $n = 7$, $r = 0.846$

Another correlation equation relating aqueous solubility to molar volume for liquid alkynes was derived by Lande and Banargee [24]

$$\log S = -0.0315(\text{MV}) + 1.26 \qquad (6.8)$$

S = mole/litre, MV = cm^3/mole, $n = 9$, $r = 0.902$

Miller and Wasik [20] studied the relationship between molar volume and solubility for chlorobenzenes and polychlorinated biphenyls

$$\log S = 3.40 - 0.0248(MV) \tag{6.9}$$

S = mole/litre, $MV = cm^3$/mole, $r = 0.92$

Miller and Wasik also derived a correlation equation relating n-octanol-water partition coefficient to molar volume for those compounds

$$\log K_{ow} = 0.49 - 0.020(MV) \tag{6.10}$$

$MV = cm^3$/mole, $r = 0.97$

In this thesis, correlations between mass partitioning of halobenzenes and these three physicochemical properties, total molecular surface area, TSA, molar volume, MV, and the substituent constant, π, are investigated. The physicochemical properties used for correlations are given in Table 6.1.2. The molar volume and total molecular surface area values are taken from Yalkowsky's paper [16], π values are calculated by using Eq. (2.22)

$$\log K_{ow} = (R'\ X_1\ X_2 \ldots X_n) = \log K_{ow}(R'H_n) + \sum_{1}^{n} \pi(X_n) \tag{2.22}$$

where $\log K_{ow}(R'\ X_1\ X_2 \ldots X_n)$ is the logarithm of the partition coefficient of the compound under consideration, $\log K_{ow}(R'H_n)$ is the logarithm of the partition coefficient of the parent structure, π is the substituent constant.

TABLE 6.1.2. The Physicochemical Properties and Logarithm of Mass Percentage in each Compartment Used for Linear Regression Analysis

NO	CHEMICAL	log % in air	log % in soil	log % in water	log % in biota	log % in suspended solids	log % in sediment	TSA A^{o2}	MV $cm^3/mole$	π
1	Benzene	1.998	-2.10	-0.28	-5.17	-4.90	2.12	109.5	89	0
2	Fluorobenzene	1.998	-2.01	-0.35	-5.12	-4.82	-2.05	113.6	94	0.14
3	Chlorobenzene	1.996	-1.22	-0.10	-4.39	-4.01	-1.23	127.1	102	0.71
4	Bromobenzene	1.99	-0.82	0.12	-4.04	-3.63	-0.85	133.1	105	0.86
5	Iodobenzene	1.98	-0.07	0.51	-3.33	-2.87	-0.1	141.9	111	1.23
6	o-Difluorobenzene	1.998	-1.81	-0.46	-4.96	-4.62	-1.84	117.7	98	0.46
7	m-Difluorobenzene	1.999	-1.96	-0.62	-5.12	-4.78	-2.00	117.7	98	0.45
8	p-Difluorobenzene	1.998	-2.00	-0.48	-4.99	-4.65	-1.87	117.7	103	0.45
9	o-Dichlorobenzene	1.99	-0.16	0.19	-3.46	-2.97	-0.19	142.7	113	1.46
10	m-Dichlorobenzene	1.99	-0.46	-0.11	-3.76	-3.26	-0.48	144.7	114	1.46
11	p-Dichlorobenzene	1.996	-0.77	-0.22	-4.05	-3.59	-0.80	144.7	118	1.25

TABLE 6.1.2 - Continued...

NO	CHEMICAL	log % in air	log % in soil	log % in water	log in biota	log % in suspended solids	log % in sediment	TSA A^{o2}	MV cm^3/mole	π
12	o-Dibromobenzene	1.95	0.63	0.49	-2.75	-2.18	0.60	153.2	121	1.94
13	m-Dibromobenzene	1.94	0.68	0.54	-2.70	-2.13	0.65	156.6	121	1.94
14	p-Dibromobenzene	1.98	0.17	0.04	-3.20	-2.63	0.15	156.6	128	1.94
15	o-Diiodobenzene	1.54	1.48	0.77	-1.97	-1.32	1.46	168.7	130	2.52
16	m-Diiodobenzene	1.68	1.39	0.69	-2.07	1.42	1.36	174.3	134	2.51
17	p-Diiodobenzene	1.54	1.49	0.78	-2.00	1.32	1.46	174.3	...	2.51
18	o-Bromochlorobenzene	1.97	0.36	0.47	-2.98	-2.45	0.33	148.0	117	1.7
19	m-Bromochlorobenzene	1.98	0.19	0.29	-3.15	-2.62	0.16	150.6	117	1.7
20	p-Bromochlorobenzene	1.99	-0.21	-0.10	-3.55	-3.02	-0.24	150.6	122	1.7
21	p-Bromoiodobenzene	1.85	1.09	0.66	-2.33	-1.72	1.06	165.5	...	2.23
22	o-Chloroiodobenzene	1.91	0.88	0.70	-2.50	-1.93	0.85	156.1	122	1.99
23	m-Chloroiodobenzene	1.92	0.79	0.61	-2.59	-2.02	0.76	159.5	...	1.99
24	p-Chloroiodobenzene	1.95	0.60	0.41	-2.79	-2.21	0.56	159.5	127	1.99

TABLE 6.1.2 - Continued.

NO	CHEMICAL	log % in air	log % in soil	log % in water	log % in biota	log % in suspended solids	log % in sediment	TSA A^{o2}	MV cm^3/mole	π
25	1,2,3-Trichloro-benzene	1.98	0.29	-0.04	-3.11	-2.52	0.26	158.3	...	2.14
26	1,2,4-Trichloro-benzene	1.98	0.15	-0.09	-3.24	-2.66	0.12	160.2	125	2.05
27	1,3,5-Trichloro-benzene	1.998	-0.70	-1.03	-4.10	-3.50	-0.72	162.2	...	2.14
28	1,2,4-Tribromo-benzene	1.56	1.50	0.46	-2.01	-1.31	1.47	176.8	...	2.85
29	1,3,5-Tribromo-benzene	1.77	1.30	0.26	-2.20	-1.51	1.27	180.2	...	2.85
30	1,2,3,4-Tetra-chlorobenzene	1.93	0.90	-0.21	-2.62	-1.91	0.87	173.8	...	2.92
31	1,2,3,5-Tetra-chlorobenzene	1.97	0.54	-0.57	-2.98	-2.27	0.51	175.8	...	2.92
32	1,2,4,5 Tetra-chlorobenzene	1.97	0.51	-0.22	-2.95	-2.29	0.48	175.8	116	2.54
33	Pentachloro-benzene	1.97	0.52	-0.73	-3.02	-2.28	0.49	189.4	136	3.06
34	Hexachloro-benzene	1.77	1.32	0.03	-2.23	-1.49	1.29	203.0	182	3.1

Specimen Calculation

As given in Table A.2.7, o-difluorobenzene has a log K_{ow} value of 2.59 and benzene has a log K_{ow} value of 2.13 and then π value for o-difluoro substituent is calculated by using Eq. (2.22)

$$\log K_{ow}(o\text{-}C_6H_4F_2) = \log K_{ow}(C_6H_6) + \sum_{1}^{2} \pi(F)$$

$$\pi = 2.59 - 2.13 = 0.46$$

The statistical calculations are performed with Casio fx-3600P scientific calculator. The results are given in Table 6.1.3. The negative slope values for the correlations with mass partitioning into the air compartment indicate an inverse relationship to these three parameters.

For benzene and 33 halobenzenes, the correlations between partitioning into the soil, sediment, biota, suspended solids compartments and these three parameters having a correlation coefficient of greater than 0.8 are good, but the correlations between partitioning into the air, water compartments and these three parameters are poor. These correlations are shown in Figure 6.1.1, Figure 6.1.2, Figure 6.1.3, Figure 6.1.4, Figure 6.1.5 and Figure 6.1.6.

When halobenzenes are divided into several groups, the most of the correlation coefficients for the soil, sediment, biota and suspended solid compartments exceed 0.9 and also some correlation coefficients for the water and air compartments exceed 0.9.

The correlations for dihalogenated benzenes are shown in Figure 6.1.7, Figure 6.1.8, Figure 6.1.9, Figure 6.1.10, Figure 6.1.11 and

TABLE 6.1.3 - Regression Analyses Using Equation $y = A + Bx^1$

CHEMICAL CLASS	y	x	n	A	B	r	No.
Benzene and Halobenzenes	log% in air	π	34	2.064	-0.084	-0.531	(1)
(includes 1-34 numbered	"	MV	25	2.336	$-3.36x10^{-3}$	-0.551	(2)
compounds)	"	TSA	34	2.417	$-3.27x10^{-3}$	-0.538	(3)
Monohalobenzenes	"	π	4	2.000	-0.016	-0.898	(4)
(includes 2-5 numbered	"	MV	4	2.099	$-1.05x10^{-3}$	-0.921	(5)
compounds)	"	TSA	4	2.071	$-6.21x10^{-4}$	-0.913	(6)
Dihalobenzenes - 1 -	"	π	12	2.156	-0.173	-0.750	(7)
(includes 6-17 numbered	"	MV	11	2.870	$-8.20x10^{-3}$	-0.658	(8)
compounds)	"	TSA	12	2.860	$-6.59x10^{-3}$	-0.751	(9)
Dihalobenzenes - 1 -	"	π	9	2.015	-0.026	-0.760	(10)
(includes 6-14 numbered	"	MV	9	2.128	$-1.29x10^{-3}$	-0.628	(11)
compounds)	"	TSA	9	2.790	$-6.20x10^{-3}$	-0.751	(12)
Dihalobenzenes - 2 -	"	π	7	2.369	-0.266	-0.946	(13)
(includes 18-24 numbered	"	MV	5	2.300	$-2.86x10^{-3}$	-0.378	(14)
compounds)	"	TSA	7	3.007	$-6.86x10^{-3}$	-0.88	(15)
Dihalobenzenes - 3 -	"	π	19	2.165	-0.154	-0.677	(16)
(includes 6-24 numbered	"	MV	16	2.771	$-7.16x10^{-3}$	-0.588	(17)
compounds)	"	TSA	19	2.784	$-5.85x10^{-3}$	-0.678	(18)
Trihalobenzenes	"	π	5	2.891	-0.429	-0.916	(19)
(includes 25-29 numbered	"	TSA	5	4.548	-0.016	-0.855	(20)
compounds)							
Chlorobenzenes (includes	"	π	12	2.058	-0.045	-0.565	(21
3,9-11,25-27,30-34	"	MV	8	2.326	$-2.93x10^{-3}$	-0.947	(22
numbered compounds)	"	TSA	12	2.301	$-2.08x10^{-3}$	-0.712	(23
Bromobenzenes (includes	"	π	6	2.278	-0.212	-0.798	(24
4,12-14,28,29 numbered	"	MV	4	2.088	$-1.04x10^{-3}$	-0.420	(25
compounds)		TSA	6	3.338	$-9.42x10^{-3}$	-0.833	(26
Benzene and Halobenzenes	log% in soil	π	34	-2.024	1.156	0.908	(27
(includes 1-34 numbered	"	MV	25	-5.936	0.049	0.796	(28
compounds)	"	TSA	34	-6.694	0.044	0.893	(29
Monohalobenzenes	"	π	4	-2.330	1.770	0.991	(30
(includes 2-5 numbered	"	MV	4	-12.78	0.114	0.997	(31
compounds)	"	TSA	4	-9.757	0.068	0.995	(32

TABLE 6.1.3 - Continued...

CHEMICAL CLASS	y	x	n	A	B	r	No.
Dihalobenzenes - 1 - (included 6-17 numbered compounds)	log% in soil	π	12	-2.698	1.640	0.994	(33)
	"	MV	11	-11.410	0.096	0.937	(34)
	"	TSA	12	-9.22	0.062	0.980	(35)
Dihalobenzenes - 2 - (included 18-24 numbered compounds)	"	π	7	-3.190	1.959	0.900	(36)
	"	MV	5	-3.214	0.030	0.300	(37)
	"	TSA	7	-8.490	0.058	0.813	(38)
Dihalobenzenes - 3 - (includes 6-24 numbered compounds)	"	π	19	-2.711	1.674	0.988	(39)
	"	MV	16	-11.22	0.095	0.914	(40)
	"	TSA	19	-9.280	0.063	0.972	(41)
Trihalobenzenes (included 25-29 numbered compunds)	"	TSA	5	-11.76	0.073	0.827	(42)
	"	π	5	-4.209	1.960	0.886	(43)
Chlorobenzenes (includes 3,9-11,25-27,30-34 numbered compounds)	"	π	12	-1.684	0.853	0.952	(44)
	"	MV	8	-3.440	0.027	0.831	(45)
	"	TSA	12	-4.840	0.031	0.929	(46)
Bromobenzenes (includes 4,12-14,28-29 numbered compounds)	"	π	6	-1.695	1.101	0.972	(47)
	"	MV	4	-6.422	0.056	0.777	(48)
	"	TSA	6	-6.781	0.046	0.949	(49)
Benzene and Halobenzenes (includes 1-34 numbered compounds)	log% in water	π	34	-0.195	0.147	0.268	(50)
	"	MV	25	-0.803	7.32×10^{-3}	0.310	(51)
	"	TSA	34	-0.785	5.55×10^{-3}	0.262	(52)
Monohalobenzenes (includes 2-5 numbered compounds)	"	π	4	-0.526	0.777	0.965	(53)
	"	MV	4	-5.153	0.050	0.979	(54)
	"	TSA	4	-3.806	0.030	0.974	(55)
Dihalobenzenes - 1 - (includes 6-17 numbered compounds)	"	π	12	-0.842	0.620	0.956	(56)
	"	MV	11	-3.943	0.035	0.868	(57)
	"	TSA	12	-3.265	0.023	0.934	(58)
Dihalobenzenes - 2 - (includes 18-24 numbered compounds)	"	π	7	-1.374	0.952	0.704	(59)
	"	MV	5	0.322	2.57×10^{-4}	3.645×10^{-3}	(60)
	"	TSA	7	-3.577	0.026	0.582	(61)
Dihalobenzenes - 3 - (includes 6-24 numbered compounds)	"	π	19	-0.856	0.649	0.925	(62)
	"	MV	16	-3.870	0.034	0.805	(63)
	"	TSA	19	-3.356	0.024	0.899	(64)
Trihalobenzenes (includes 25-29 compounds)	"	π	5	-2.390	0.956	0.681	(65)
	"	TSA	5	-5.765	0.034	0.603	(66)

TABLE 6.1.3 - Continued...

CHEMICAL CLASS	y	x	n	A	B	r	No.
Chlorobenzenes (includes 3, 9-11,25-27,30-34 numbered compounds)	log% in water	π	12	0.063	-0.150	-0.342	(67)
	"	MV	8	-0.130	-2.13x10^{-4}	-0.020	(68)
	"	TSA	12	0.477	-4.51x10^{-3}	-0.280	(69)
Bromobenzenes (includes 4,12-14,28,29 numbered compounds)	"	π	6	0.102	0.104	0.370	(70)
	"	MV	4	-0.135	3.64x10^{-3}	0.140	(71)
	"	TSA	6	-0.269	3.68x10^{-3}	0.303	(72)
Benzene and Halobenzenes (includes 1-34 numbered compounds)	log% in biota	π	34	-5.086	0.996	0.884	(73)
	"	MV	25	-8.478	0.042	0.780	(74)
	"	TSA	34	-9.108	0.038	0.869	(75)
Monohalobenzenes (includes 2-5 numbered compounds)	"	π	4	-5.418	1.630	0.991	(76)
	"	MV	4	-15.04	0.105	0.997	(77)
	"	TSA	4	-12.25	0.062	0.994	(78)
Dihalobenzenes - 1 - (includes 6-17 numbered compounds)	"	π	12	-5.728	1.467	0.992	(79)
	"	MV	11	-13.50	0.086	0.936	(80)
	"	TSA	12	-11.54	0.055	0.977	(81)
Dihalobenzenes - 2 - (includes 18-24 numbered compounds)	"	π	7	-6.277	1.808	0.884	(82)
	"	MV	5	-5.984	0.025	0.263	(83)
	"	TSA	7	-11.11	0.053	0.793	(84)
Dihalobenzenes - 3 - (includes 6-24 numbered compounds)	"	π	19	-5.743	1.497	0.985	(85)
	"	MV	16	-13.33	0.085	0.910	(86)
	"	TSA	19	-11.61	0.056	0.967	(87)
Trihalobenzenes (includes 25-29 numbered compounds)	"	π	5	-7.296	1.814	0.875	(88)
	"	TSA	5	-14.24	0.068	0.810	(89)
Chlorobenzenes (includes 3,9-11,25-27,30-34 numbered compounds)	"	π	12	-4.831	0.701	0.863	(90)
	"	MV	8	-6.282	0.023	0.833	(91)
	"	TSA	12	-7.458	0.025	0.850	(92)
Bromobenzenes (includes 4,12-14,28,29 numbered compounds)	"	π	6	-4.793	0.958	0.965	(93)
	"	MV	4	-8.88	0.048	0.755	(94)
	"	TSA	6	-9.205	0.040	0.940	(95)
Benzene and Halobenzenes (includes 1-34 numbered compounds)	log% in sus.	π	34	-4.805	1.142	0.909	(96)
	" solids	MV	25	-8.683	0.048	0.799	(97)
	"	TSA	34	-9.417	0.043	0.893	(98)
Monohalobenzenes (includes 2-5 numbered compounds)	"	π	4	-5.12	1.758	0.992	(99)
	"	MV	4	-15.49	0.113	0.997	(100)
	"	TSA	4	-12.49	0.067	0.995	(101)

TABLE 6.1.3 - Continued...

CHEMICAL CLASS	y	x	n	A	B	r	No.
Dihalobenzenes - 1 - (includes 6-17 numbered compounds)	log% in sus.sol.	π	12	-5.455	1.616	0.993	(102)
	"	MV	11	-14.01	0.094	0.939	(103)
	"	TSA	12	-11.85	0.061	0.979	(104)
Dihalobenzenes - 2 - (includes 18-24 numbered compounds)	"	π	7	-6.003	1.959	0.900	(105)
	"	MV	5	-6.024	0.030	0.230	(106)
	"	TSA	7	-11.30	0.058	0.813	(107)
Dihalobenzenes - 3 - (includes 6-24 numbered compounds)	"	π	19	-5.469	1.647	0.987	(108)
	"	MV	16	-13.83	0.093	0.915	(109)
	"	TSA	19	-11.92	0.061	0.970	(110)
Trihalobenzenes (includes 25-29 numbered compounds)	"	π	5	-6.915	1.913	0.885	(111)
	"	TSA	5	-14.32	0.072	0.829	(112)
Chlorobenzenes (includes 3,9-11,25-27,30-34 numbered compounds)	"	π	12	-4.560	0.853	0.901	(113)
	"	MV	8	-6.230	0.027	0.829	(114)
	"	TSA	12	-7.727	0.031	0.884	(115)
Bromobenzenes (includes 4,12-14,28,29 numbered compounds)	"	π	5	-4.170	0.957	0.922	(116)
	"	MV	3	6.056	-0.067	-0.996	(117)
	"	TSA	5	-7.892	0.036	0.887	(118)
Benzene and Halobenzenes (includes 1-34 numbered compounds)	log% in sed.	π	34	-2.032	1.147	0.908	(119)
	"	MV	25	-5.922	0.049	0.798	(120)
	"	TSA	34	-6.664	0.044	0.893	(121)
Monohalobenzenes (includes 2-5 numbered compounds)	"	π	4	-2.365	1.779	0.993	(122)
	"	MV	4	-12.85	0.115	0.998	(123)
	"	TSA	4	-9.820	0.068	0.996	(124)
Dihalobenzenes - 1 - (includes 6-17 numbered compounds)	"	π	12	-2.678	1.620	0.993	(125)
	"	MV	11	-11.29	0.095	0.940	(126)
	"	TSA	12	-9.110	0.061	0.980	(127)
Dihalobenzenes - 2 - (includes 18-24 numbered compounds)	"	π	7	-3.218	1.955	0.898	(128)
	"	MV	5	-3.142	0.029	0.292	(129)
	"	TSA	7	-8.500	0.058	0.811	(130)
Dihalobenzenes - 3 - (includes 6-24 numbered compounds)	"	π	19	-2.692	1.65	0.987	(131)
	"	MV	16	-11.09	0.094	0.916	(132)
	"	TSA	19	-9.167	0.062	0.971	(133)
Trihalobenzenes (includes 25-29 numbered compounds)	"	π	5	-4.227	1.956	0.887	(134)
	"	TSA	5	-11.77	0.073	0.828	(135)

TABLE 6.1.3 - Continued.

CHEMICAL CLASS	y	x	n	A	B	r	No.
Chlorobenzenes	log% in sedim.	π	12	-1.755	0.838	0.903	(136)
(includes 3,9-11,25-27,	"	MV	8	-3.927	0.026	0.819	(137)
numbered compounds)	"	TSA	12	-4.836	0.03	0.879	(138)
Bromobenzenes	"	π	6	-1.723	1.101	0.972	(139)
(includes 4,12-14,28,	"	MV	4	-6.474	0.056	0.780	(140)
29 numbered compounds)	"	TSA	6	-6.808	0.046	0.949	(141)

Linear Regression

$$y = A + Bx$$

$$B = \frac{n.\Sigma xy - \Sigma x.\Sigma y}{n\Sigma x^2 - (\Sigma x)^2}$$

$$A = \frac{\Sigma y - B\ \Sigma x}{n}$$

$$r = \frac{n.\Sigma xy - \Sigma x.\Sigma y}{\sqrt{\{n.\Sigma x^2 - (\Sigma x)^2\}\{n.\Sigma y^2 - (\Sigma y)^2\}}}$$

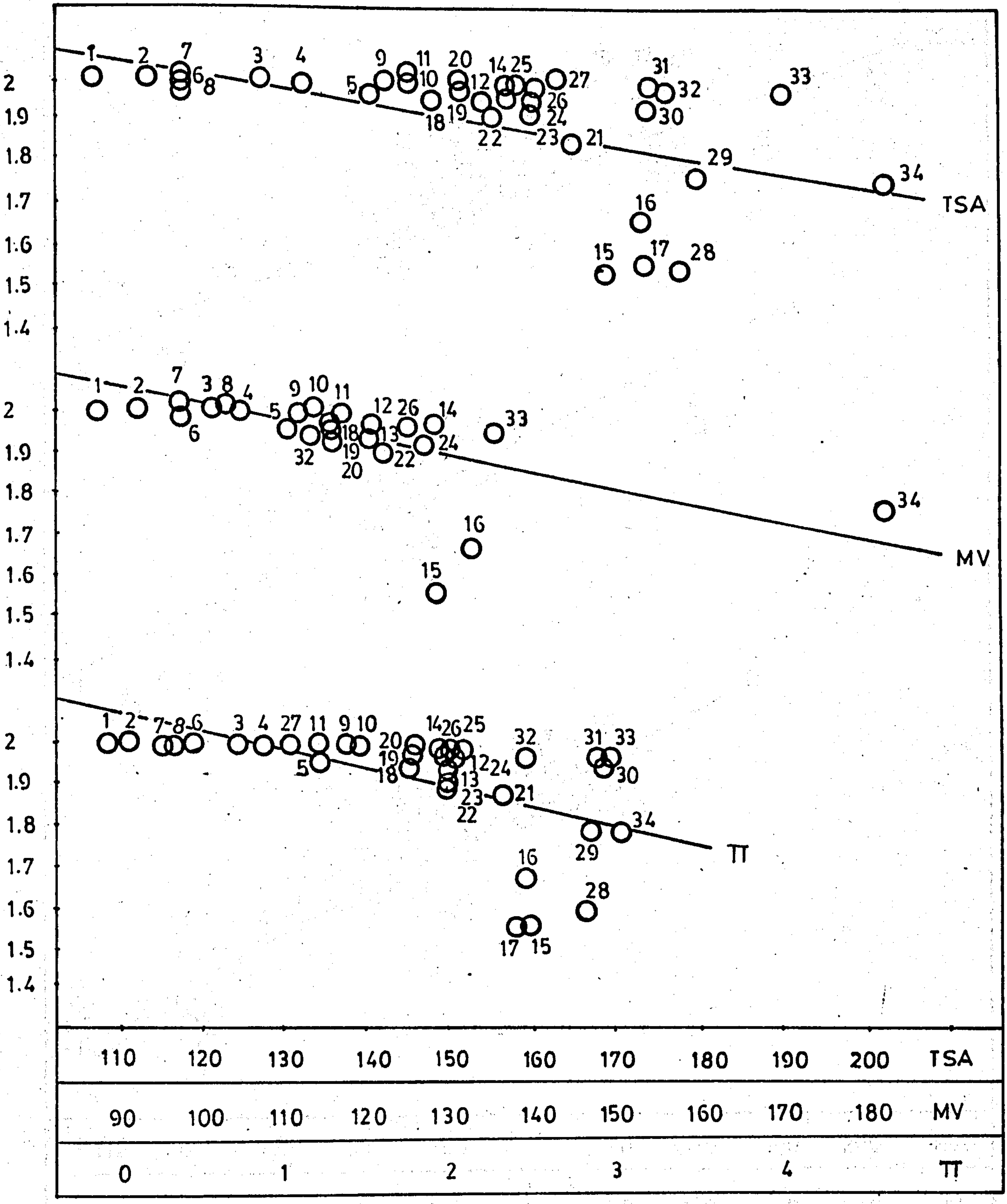


FIGURE 6.1.1. Plots of logarithm of mass partitioning into the air compartment versus total molecular surface area TSA, molar volume MV, and π substituent constant for halobenzenes

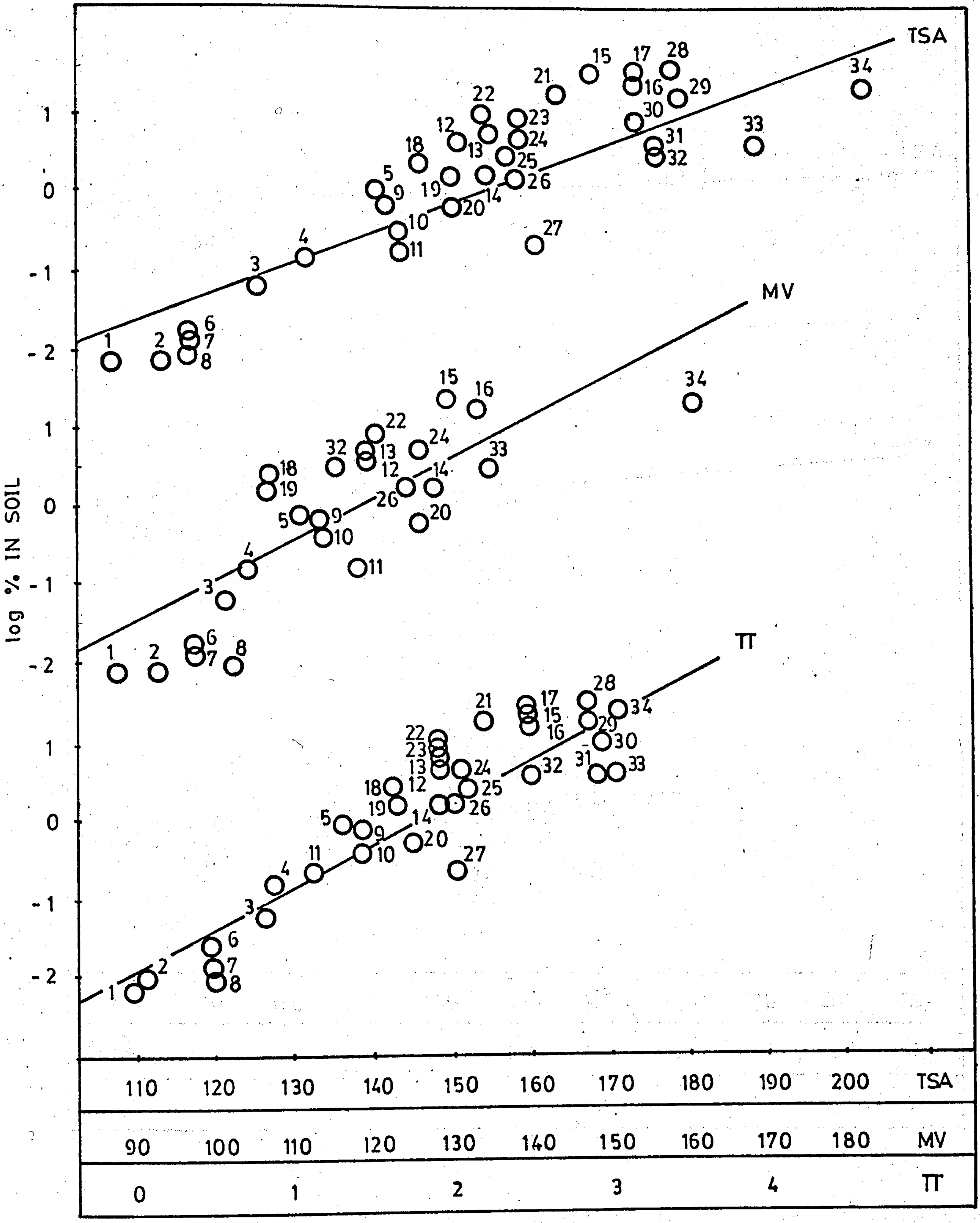


FIGURE 6.1.2. Plots of logarithm of mass partitioning into the soil compartment versus total molecular surface area TSA, molar volume MV, and π substituent constant for halobenzenes

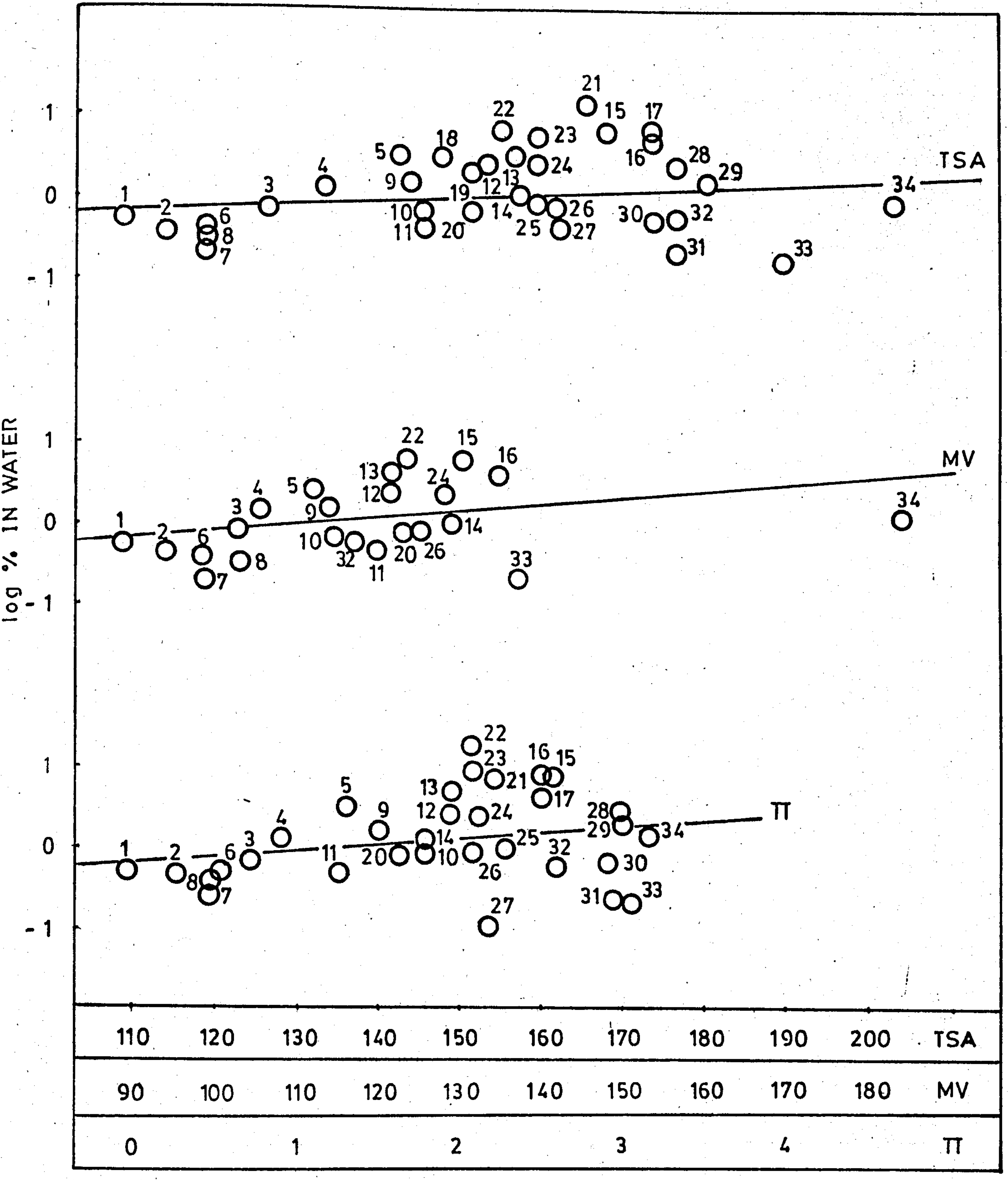


FIGURE 6.1.3. Plots of logarithm of mass partitioning into the water compartment versus total molecular surface area TSA, molar volume MV, and TT substituent constant for halobenzenes

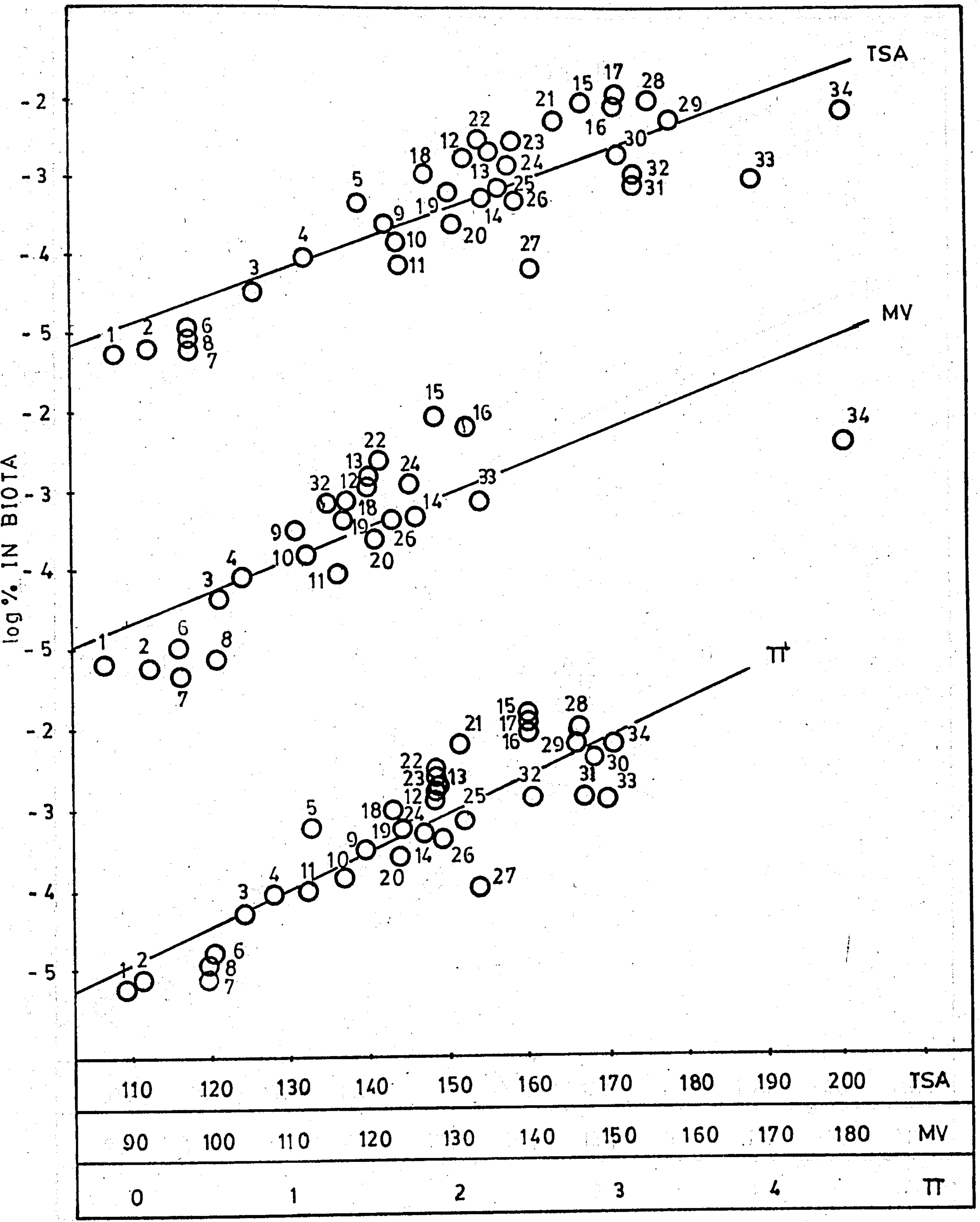


FIGURE 6.1.4. Plots of logarithm of mass partitioning into the biota compartment versus total molecular surface area TSA, molar volume MV, and π substituent constant for halobenzenes

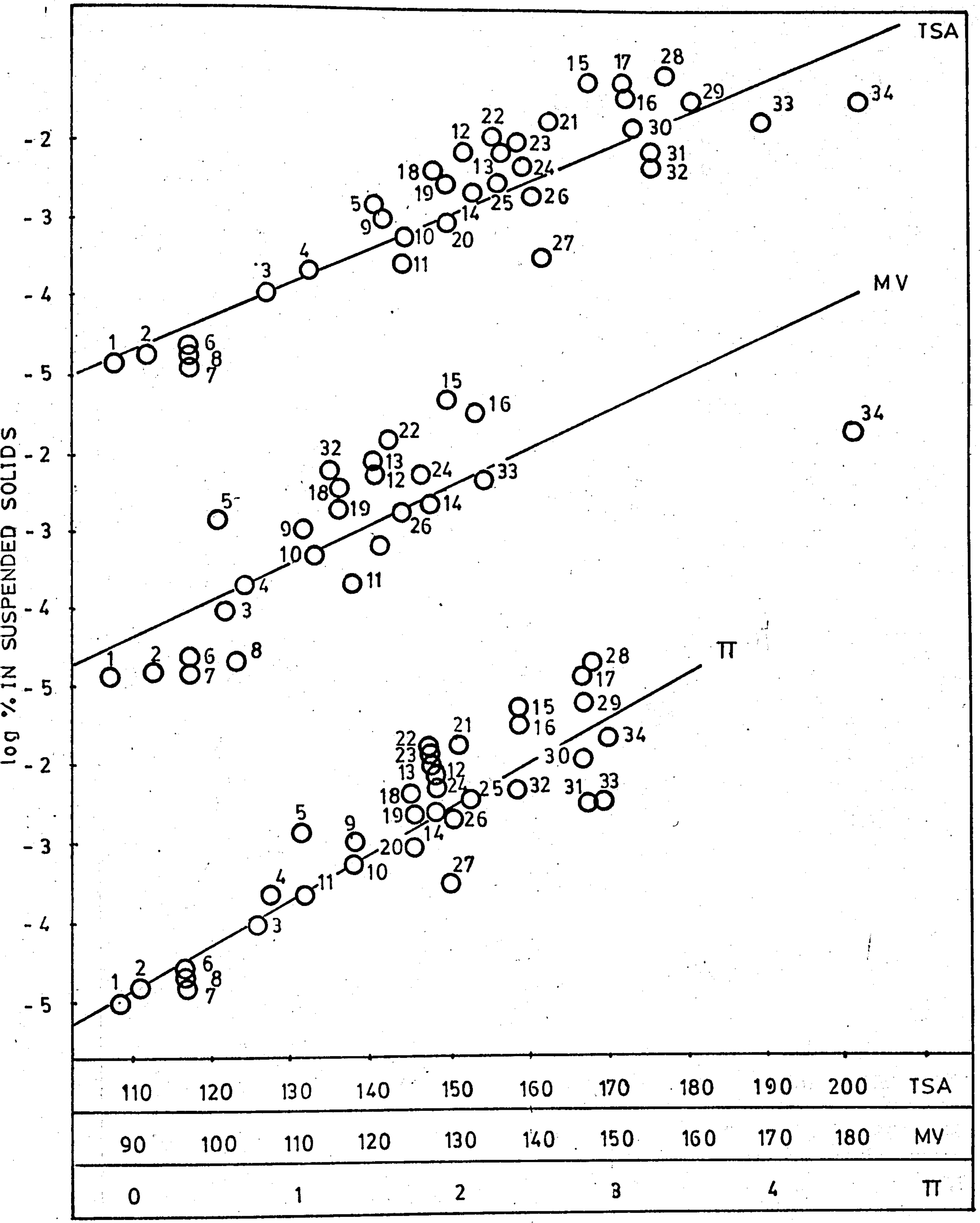


FIGURE 6.1.5. Plots of logarithm of mass partitioning into the suspended solids compartment versus total molecular surface area TSA, molar volume MV, and π substituent constant for halobenzenes

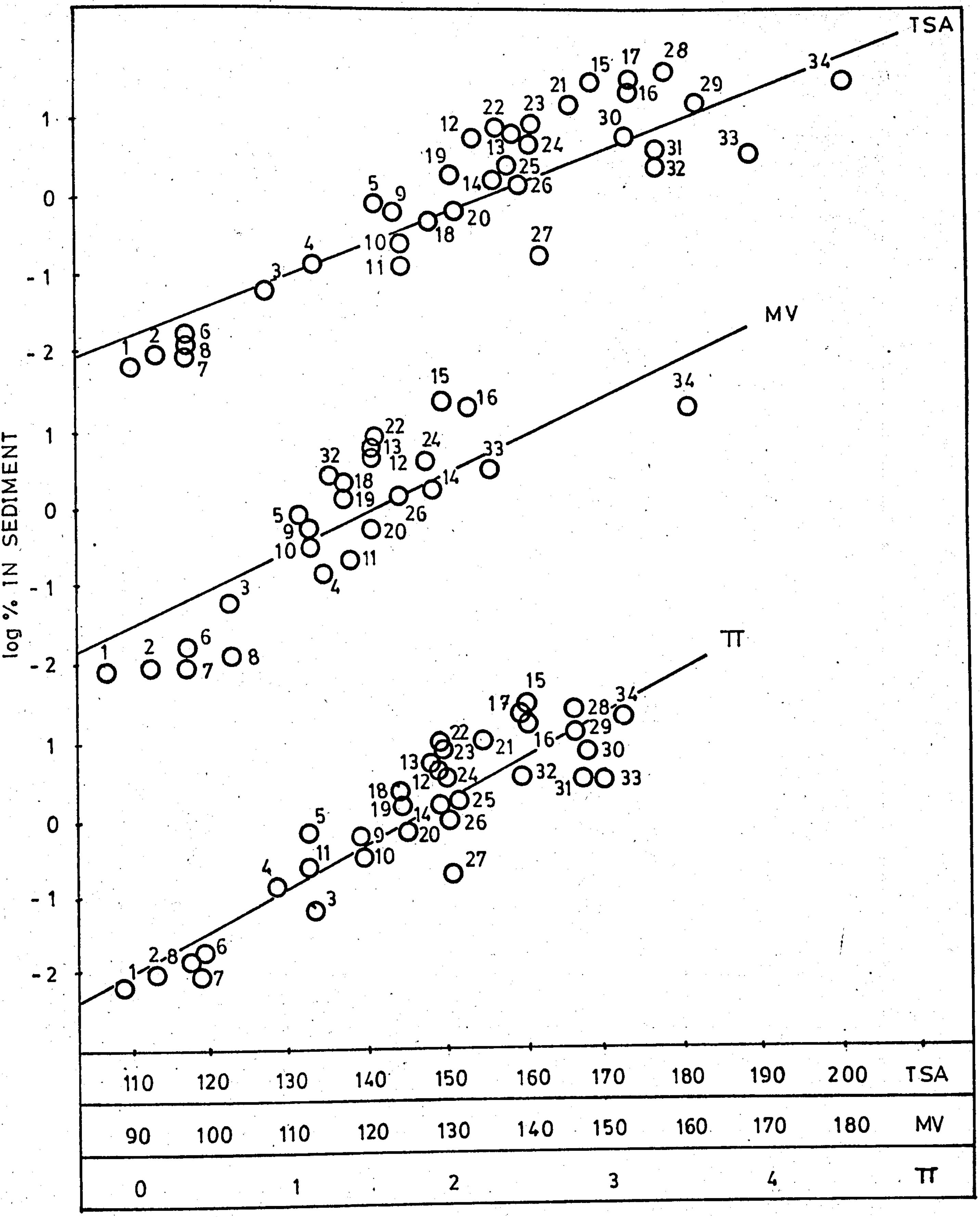


FIGURE 6.1.6. Plots of logarithm of mass partitioning into the sediment compartment versus total molecular surface area TSA, molar volume MV, and TT substituent constant for halobenzenes.

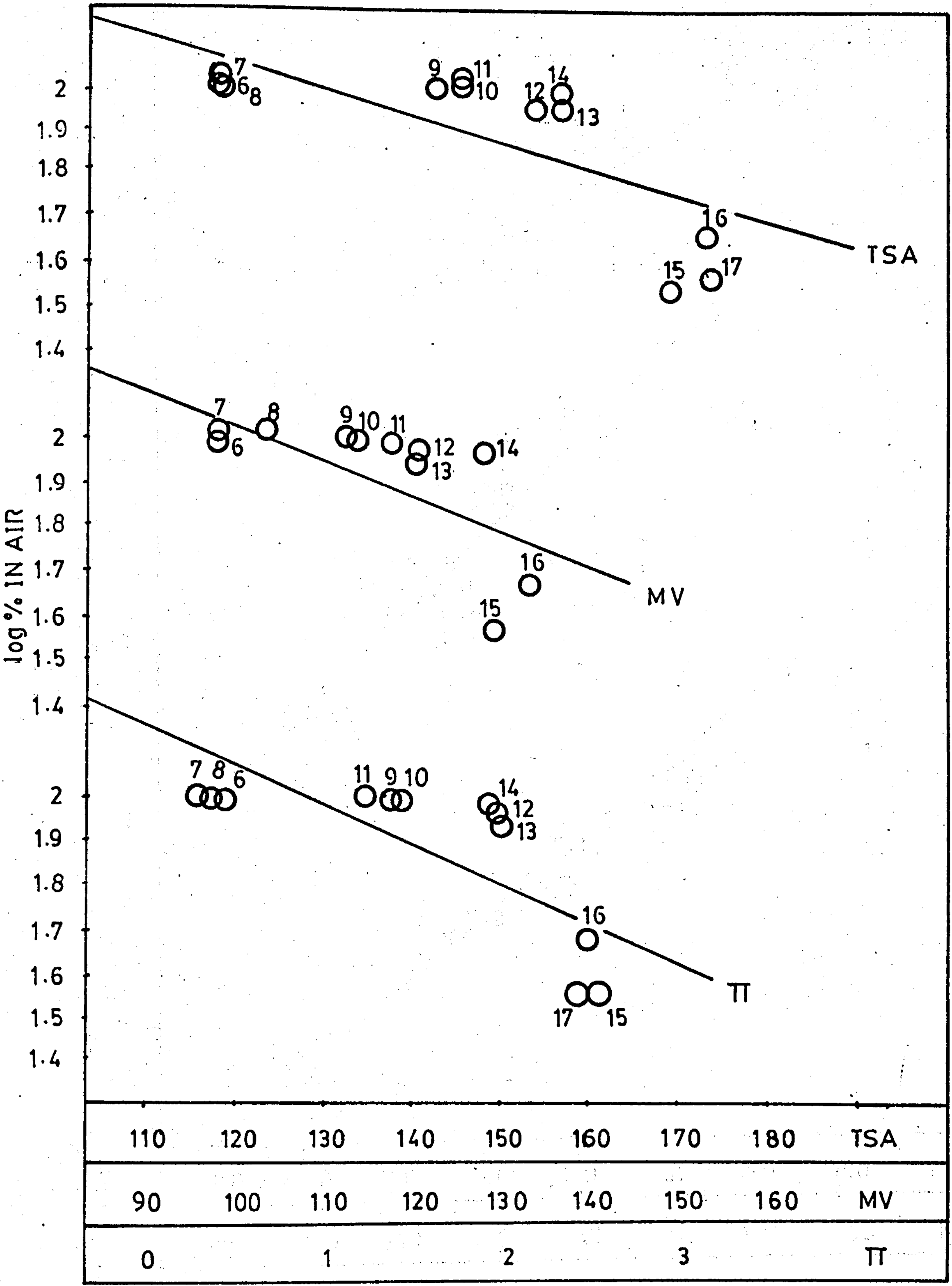


FIGURE 6.1.7. Plots of logarithm of mass partitioning into the air compartment versus total molecular surface area TSA, molar volume MV, and Π substituent constant for dihalogenated benzenes

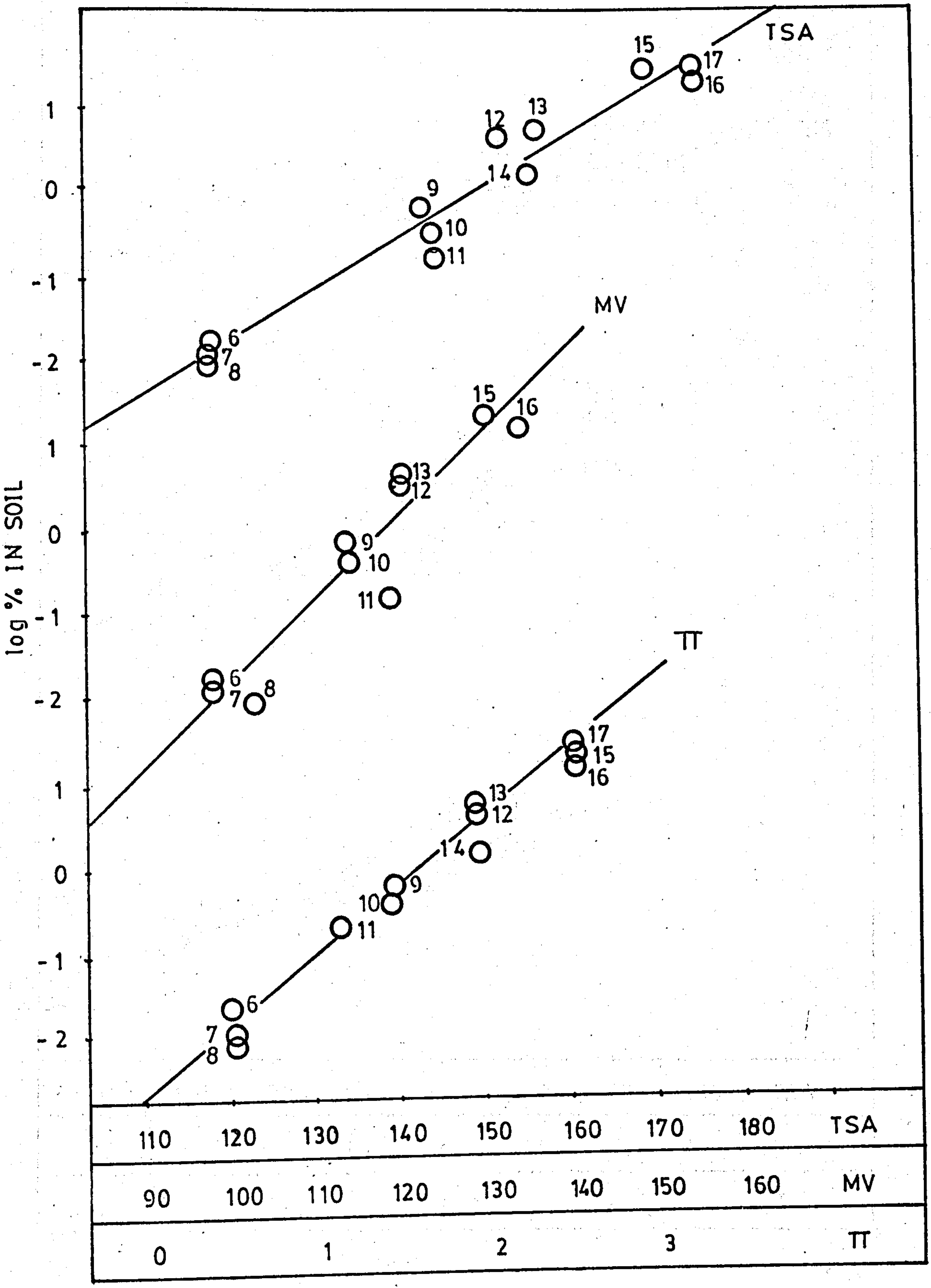


FIGURE 6.1.8. Plots of logarithm of mass partitioning into the soil compartment versus total molecular surface area TSA, molar volume MV, and π substituent constant for dihalogenated benzenes

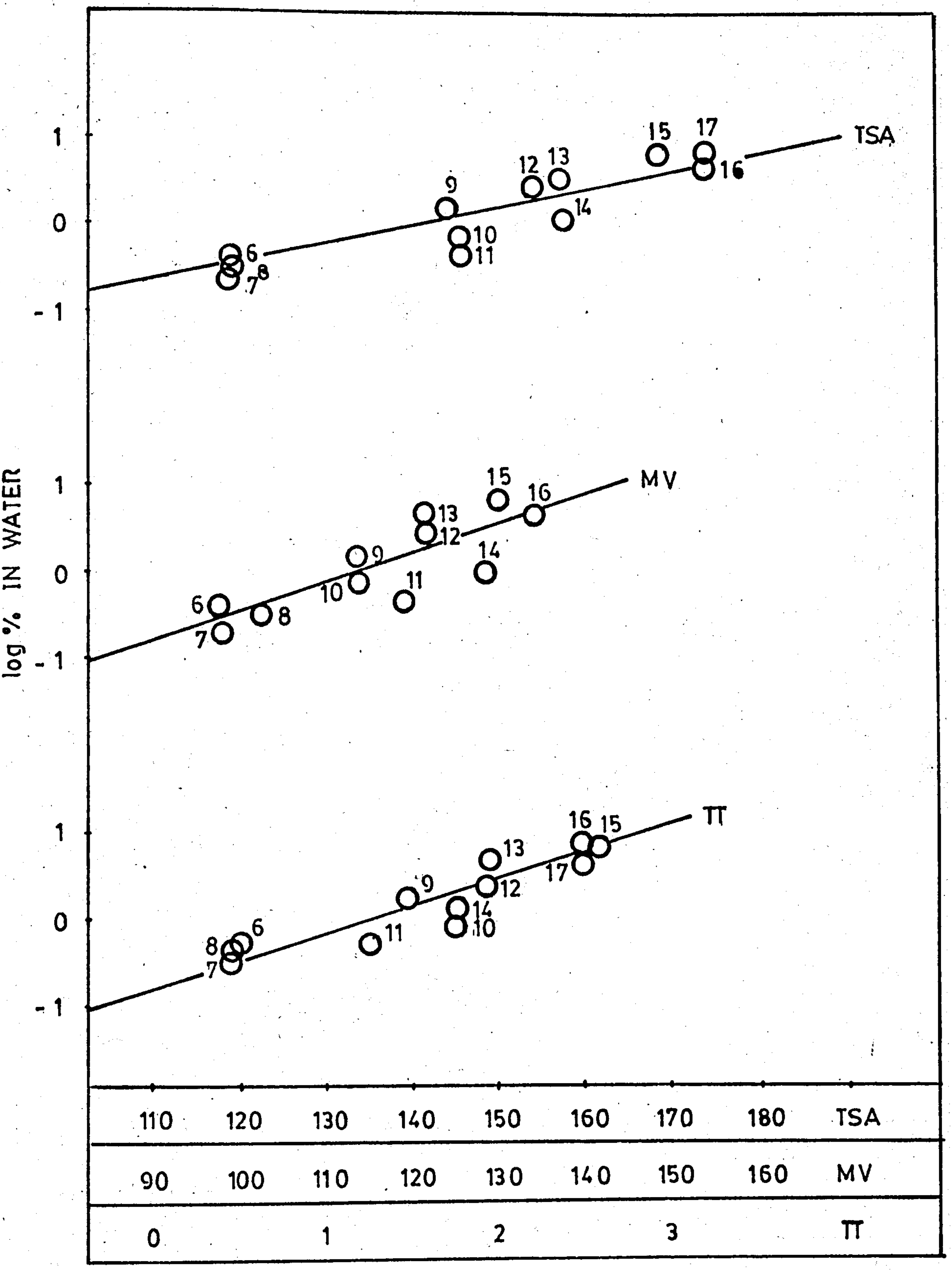


FIGURE 6.1.9. Plots of logarithm of mass partitioning into the water compartment versus total molecular surface area TSA, molar volume MV, and Π substituent constant for dihalogenated benzenes

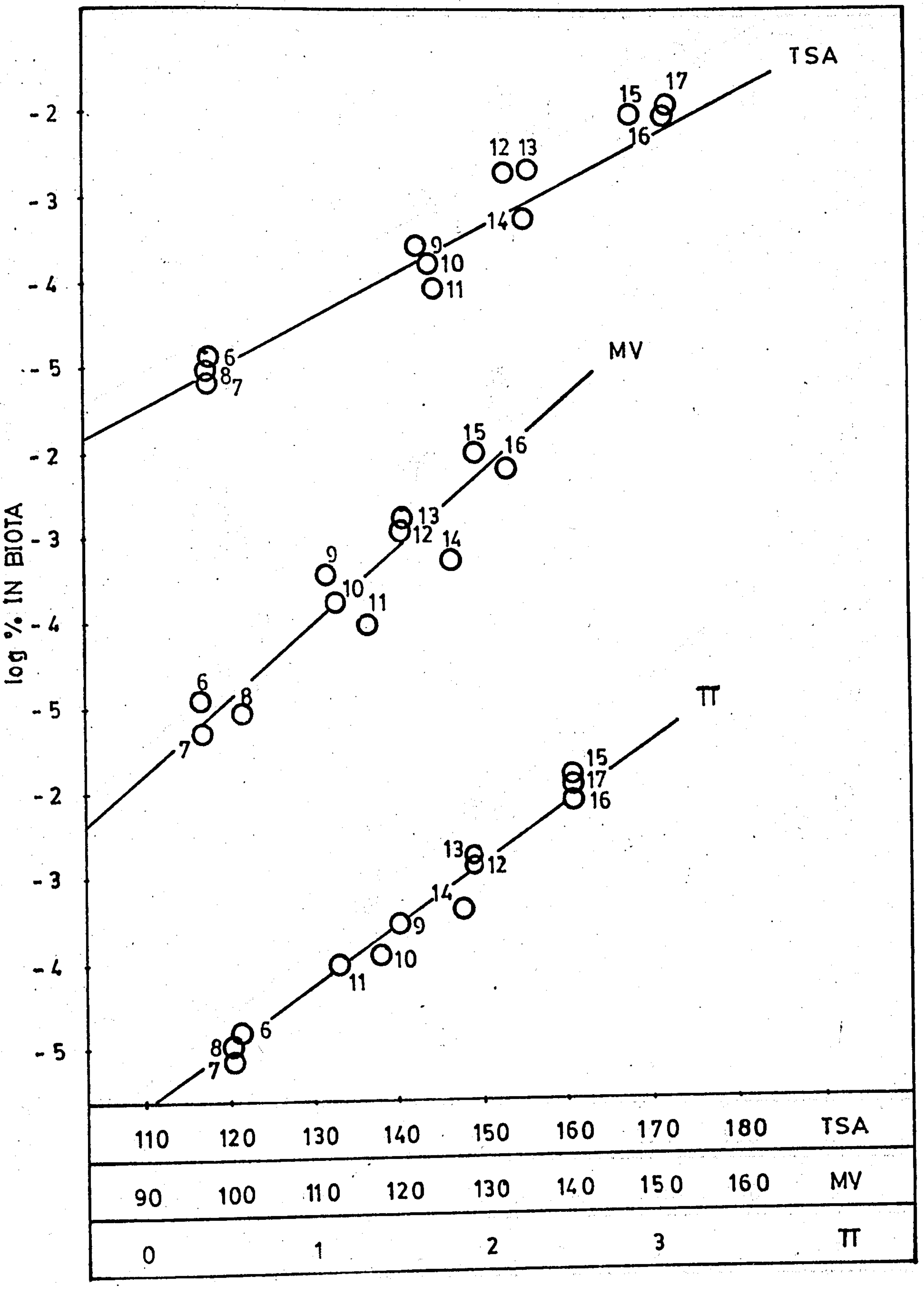


FIGURE 6.1.10 Plots of logarithm of mass partitioning into the biota compartment versus total molecular surface area TSA, molar volume MV, and TT substituent constant, for dihalogenated benzenes

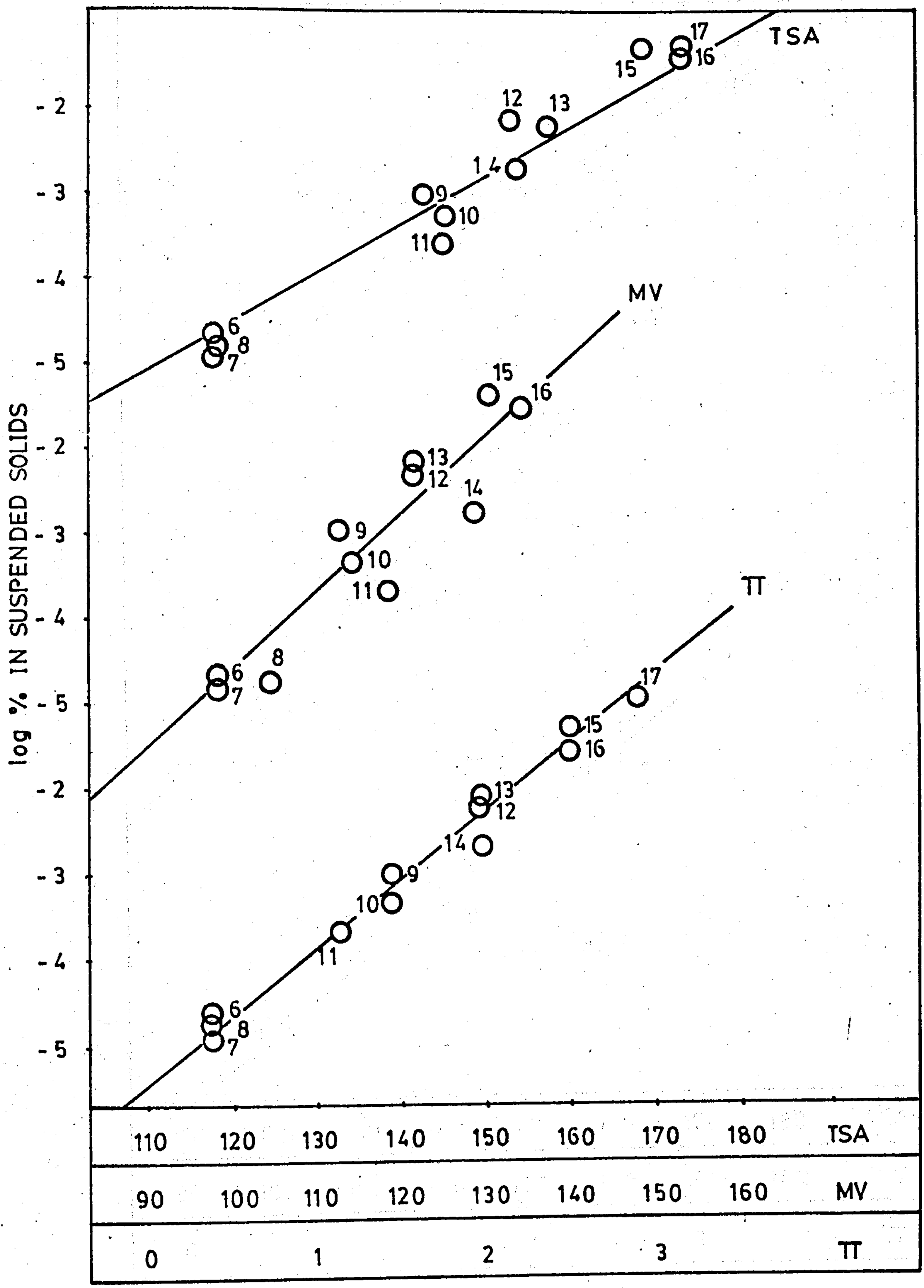


FIGURE 6.1.11 Plots of logarithm of mass partitioning into the suspended solids compartment versus total molecular surface area TSA, molar volume MV, and TT substituent constant for dihalogenated benzenes

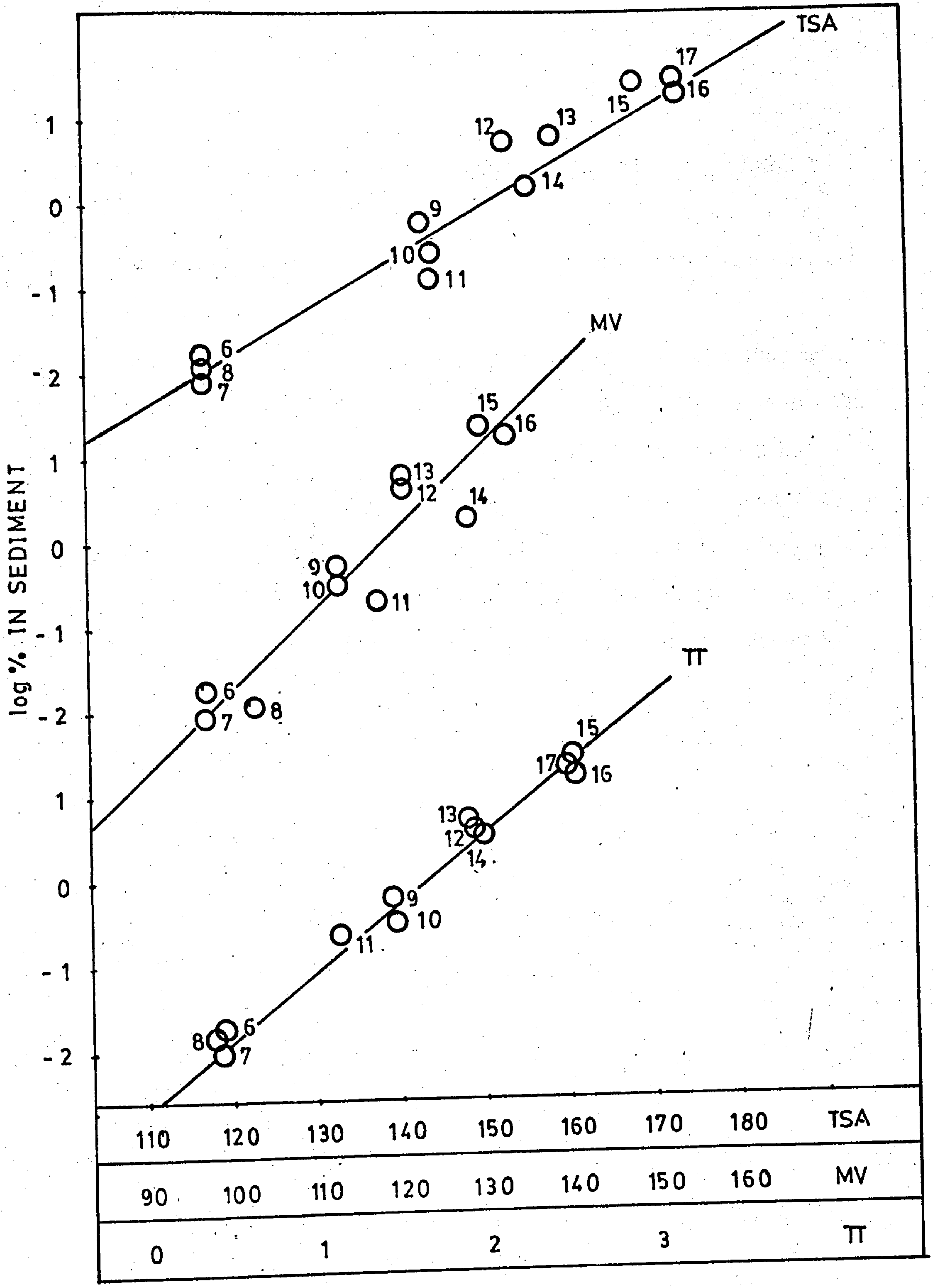


FIGURE 6.1.12. Plots of logarithm of mass partitioning into the sediment compartment versus total molecular surface are TSA, molar volume MV, and TT substituent constant for dihalogenated benzenes

Figure 6.1.12. These correlations except for the air compartment with a correlation coefficient of greater than 0.9 are very good. There is a poorer correlation between partitioning into the air compartment and these three parameters.

The comparison of the calculated equilibrium distributions of dihalogenated benzenes from TSA, MV and π by using the correlation equations obtained during this study with those calculated through Mackay's Level I Fugacity Model is given in Table 6.1.4. As can be seen also in Figure 6.1.13, Figure 6.1.14, Figure 6.1.15, Figure 6.1.16, Figure 6.1.17 and Figure 6.1.18, these values calculated from TSA, MV and π values are in agreement with those calculated through Mackay's Level I Fugacity Model.

TABLE 6.1.4 - Comparison of the Calculated Equilibrium Distributions of Dihalogenated Benzenes from π, MV, TSA by Using Correlation Equations Obtained During this Study with Those Calculated Through Mackay's Level I Fugacity Model.

CHEMICAL	log % in air		log % in soil		log % in water		log % in biota		log % in suspended solids		log % in sediment	
o-Difluorobenzene	1.998	Level I	-1.81	Level I	-0.46	Level I	-4.96	Level I	-4.62	Level I	-1.84	Level I
	2.076	Eq. 7	-0.30	Eq. 33	-0.56	Eq. 56	-5.05	Eq. 79	-4.71	Eq. 102	-1.93	Eq. 125
	2.060	Eq. 8	-2.00	Eq. 34	-0.55	Eq. 57	-5.11	Eq. 80	-4.77	Eq. 103	-1.99	Eq. 126
	2.079	Eq. 9	-1.95	Eq. 35	-0.55	Eq. 58	-5.06	Eq. 81	-4.71	Eq. 104	-1.94	Eq. 127
m-Difluorobenzene	1.999	Level I	-1.96	Level I	-0.62	Level I	-5.12	Level I	-4.78	Level I	-2.00	Level I
	2.078	Eq. 7	-1.96	Eq. 33	-0.56	Eq. 56	-5.07	Eq. 79	-4.73	Eq. 102	-1.95	Eq. 125
	2.060	Eq. 8	-2.00	Eq. 34	-0.55	Eq. 57	-5.11	Eq. 80	-4.77	Eq. 103	-1.99	Eq. 126
	2.079	Eq. 9	-1.95	Eq. 35	-0.55	Eq. 58	-5.06	Eq. 81	-4.71	Eq. 104	-1.94	Eq. 127
p-Difluorobenzene	1.998	Level I	-2.00	Level I	-0.48	Level I	-4.99	Level I	-4.65	Level I	-1.87	Level I
	2.078	Eq. 7	-1.96	Eq. 33	-0.56	Eq. 56	-5.07	Eq. 79	-4.73	Eq. 102	-1.95	Eq. 125
	2.023	Eq. 8	-1.52	Eq. 34	-0.38	Eq. 57	-4.68	Eq. 80	-4.30	Eq. 103	-1.52	Eq. 126
	2.079	Eq. 9	-1.95	Eq. 35	-0.55	Eq. 58	-5.06	Eq. 81	-4.71	Eq. 104	-1.94	Eq. 127

TABLE 6.1.4 - Continued...

CHEMICAL	log % in air		log % in soil		log % in water		log % in biota		log % in suspended solids		log % in sediment	
o-Dichlorobenzene	1.99	Level I	-0.16	Level I	0.19	Level I	-3.46	Level I	-2.97	Level I	-0.19	Level I
	1.90	Eq. 7	-0.30	Eq. 33	0.06	Eq. 56	-3.59	Eq. 79	-3.10	Eq. 102	-0.31	Eq. 125
	1.94	Eq. 8	-0.56	Eq. 34	-0.04	Eq. 57	-3.82	Eq. 80	-3.36	Eq. 103	-0.57	Eq. 126
	1.91	Eq. 9	-0.40	Eq. 35	0.03	Eq. 58	-3.68	Eq. 81	-3.20	Eq. 104	-0.41	Eq. 127
m-Dichlorobenzene	1.99	Level I	-0.46	Level I	-0.11	Level I	-3.76	Level I	-3.26	Level I	-0.48	Level I
	1.90	Eq. 7	-0.30	Eq. 33	0.06	Eq. 56	-3.59	Eq. 79	-3.10	Eq. 102	-0.31	Eq. 125
	1.93	Eq. 8	-0.47	Eq. 34	-1.97×10^{-4}	Eq. 57	-3.74	Eq. 80	-3.26	Eq. 103	-0.48	Eq. 126
	1.90	Eq. 9	-0.28	Eq. 35	0.07	Eq. 58	-3.57	Eq. 81	-3.07	Eq. 104	-0.29	Eq. 127
p-Dichlorobenzene	2.00	Level I	-0.77	Level I	-0.22	Level I	-4.05	Level I	-3.59	Level I	-0.80	Level I
	1.94	Eq. 7	-0.64	Eq. 33	-0.06	Eq. 56	-3.89	Eq. 79	-3.42	Eq. 102	-0.65	Eq. 125
	1.90	Eq. 8	-0.08	Eq. 34	0.14	Eq. 57	-3.39	Eq. 80	-2.88	Eq. 103	-0.1	Eq. 126
	1.90	Eq. 9	-0.28	Eq. 35	0.07	Eq. 58	-3.57	Eq. 81	-3.07	Eq. 104	-0.29	Eq. 127

TABLE 6.1.4 - Continued...

CHEMICAL	log % in air		log % in soil		log % in water		log % in biota		log % in suspended solids		log % in sediment	
o-Dibromobenzene	1.95	Level I	0.63	Level I	0.49	Level I	-2.75	Level I	-2.18	Level I	0.60	Level I
	1.82	Eq. 7	0.49	Eq. 33	0.36	Eq. 56	-2.88	Eq. 79	-2.32	Eq. 102	0.47	Eq. 125
	1.88	Eq. 8	0.21	Eq. 34	0.24	Eq. 57	-3.14	Eq. 80	-2.60	Eq. 103	0.19	Eq. 126
	1.85	Eq. 9	0.25	Eq. 35	0.27	Eq. 58	-3.10	Eq. 81	-2.56	Eq. 104	0.23	Eq. 127
m-Dibromobenzene	1.94	Level I	0.68	Level I	0.54	Level I	-2.70	Level I	-2.13	Level I	0.65	Level I
	1.82	Eq. 7	0.49	Eq. 33	0.36	Eq. 56	-2.88	Eq. 79	-2.32	Eq. 102	0.67	Eq. 125
	1.88	Eq. 8	0.21	Eq. 34	0.24	Eq. 57	-3.14	Eq. 80	-2.60	Eq. 103	0.19	Eq. 126
	1.82	Eq. 9	0.46	Eq. 35	0.35	Eq. 58	-2.91	Eq. 81	-2.35	Eq. 104	0.44	Eq. 127
p-Dibromobenzene	1.98	Level I	0.17	Level I	0.04	Level I	-3.20	Level I	-2.63	Level I	0.15	Level I
	1.82	Eq. 7	0.49	Eq. 33	0.36	Eq. 56	-2.88	Eq. 79	-2.32	Eq. 102	0.47	Eq. 125
	1.82	Eq. 8	0.88	Eq. 34	0.48	Eq. 57	-2.53	Eq. 80	-1.94	Eq. 103	0.85	Eq. 126
	1.82	Eq. 9	0.46	Eq. 35	0.35	Eq. 58	-2.91	Eq. 81	-2.35	Eq. 104	0.44	Eq. 127

TABLE 6.1.4 - Continued...

CHEMICAL	log % in air		log % in soil		log % in water		log % in biota		log % in suspended solids		log % in sediment	
o-Diiodobenzene	1.54	Level I	1.48	Level I	0.77	Level I	-1.97	Level I	-1.32	Level I	1.46	Level I
	1.72	Eq. 7	1.45	Eq. 33	0.72	Eq. 56	-2.03	Eq. 79	-1.38	Eq. 102	1.41	Eq. 125
	1.80	Eq. 8	1.07	Eq. 34	0.55	Eq. 57	-2.36	Eq. 80	-1.75	Eq. 103	1.04	Eq. 126
	1.74	Eq. 9	1.21	Eq. 35	0.63	Eq. 58	-2.25	Eq. 81	-1.62	Eq. 104	1.17	Eq. 127
m-Diiodobenzene	1.68	Level I	1.39	Level I	0.69	Level I	-2.07	Level I	-1.47	Level I	1.36	Level I
	1.72	Eq. 7	1.43	Eq. 33	0.71	Eq. 56	-2.05	Eq. 79	-1.40	Eq. 102	1.39	Eq. 125
	1.77	Eq. 8	1.46	Eq. 34	0.69	Eq. 57	-2.02	Eq. 80	-1.37	Eq. 103	1.42	Eq. 126
	1.71	Eq. 9	1.55	Eq. 35	0.75	Eq. 58	-1.94	Eq. 81	-1.28	Eq. 104	1.51	Eq. 127
p-Diiodobenzene	1.54	Level I	1.49	Level I	0.78	Level I	-2.00	Level I	-1.32	Level I	1.46	Level I
	1.72	Eq. 7	1.43	Eq. 33	0.71	Eq. 56	-2.05	Eq. 79	-1.40	Eq. 102	1.39	Eq. 125
	1.71	Eq. 9	1.55	Eq. 35	0.75	Eq. 58	1.94	Eq. 81	-1.28	Eq. 104	1.51	Eq. 127

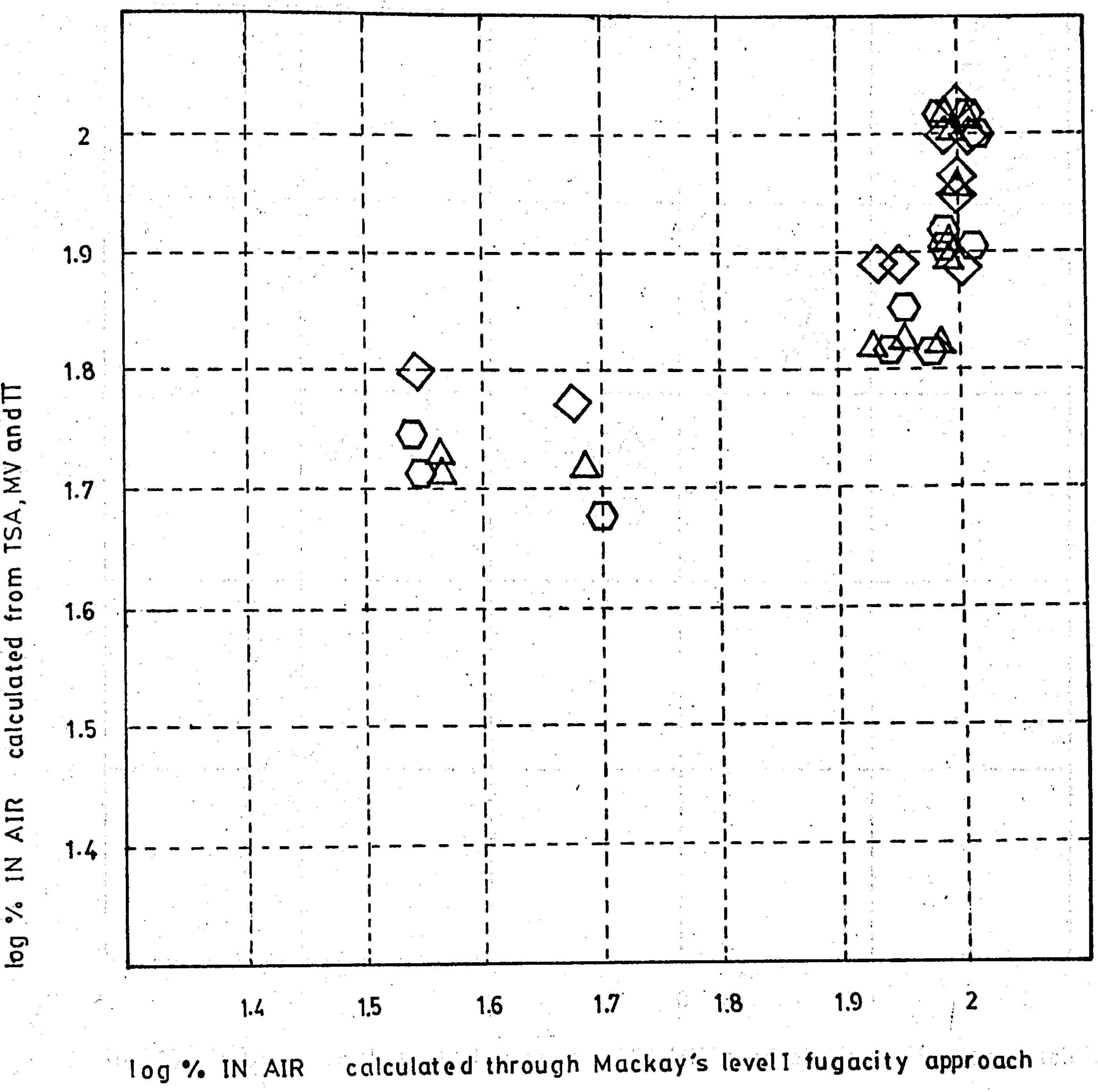


FIGURE 6.1.13. Plots of logarithm of mass partitioning into the air compartment calculated from total surface area TSA by equation 9 (⬡), from molar volume MV by equation 8 (◇), from π substituent constant by equation 7 (△) versus those calculated through Mackay's level I fugacity approach for dihalogenated benzenes

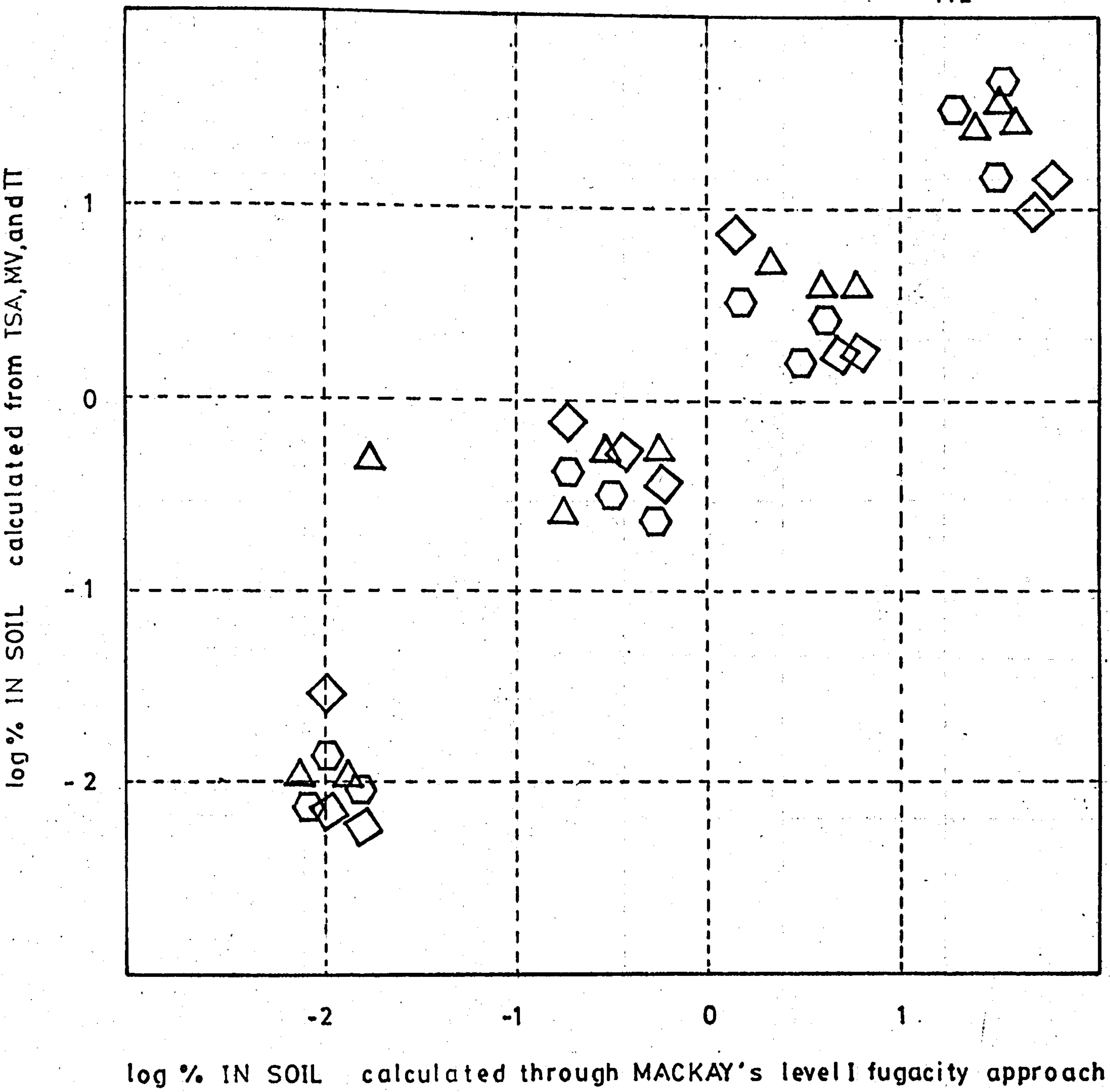


FIGURE 6.1.14. Plots of logarithm of mass partitioning into the soil compartment calculated from total molecular surface area TSA by equation 35 (⬡), from molar volume MV by equation 34 (◇), from π substituent constant by equation 33 (△) versus those calculated through Mackay's level I fugacity approach for dihalogenated benzenes

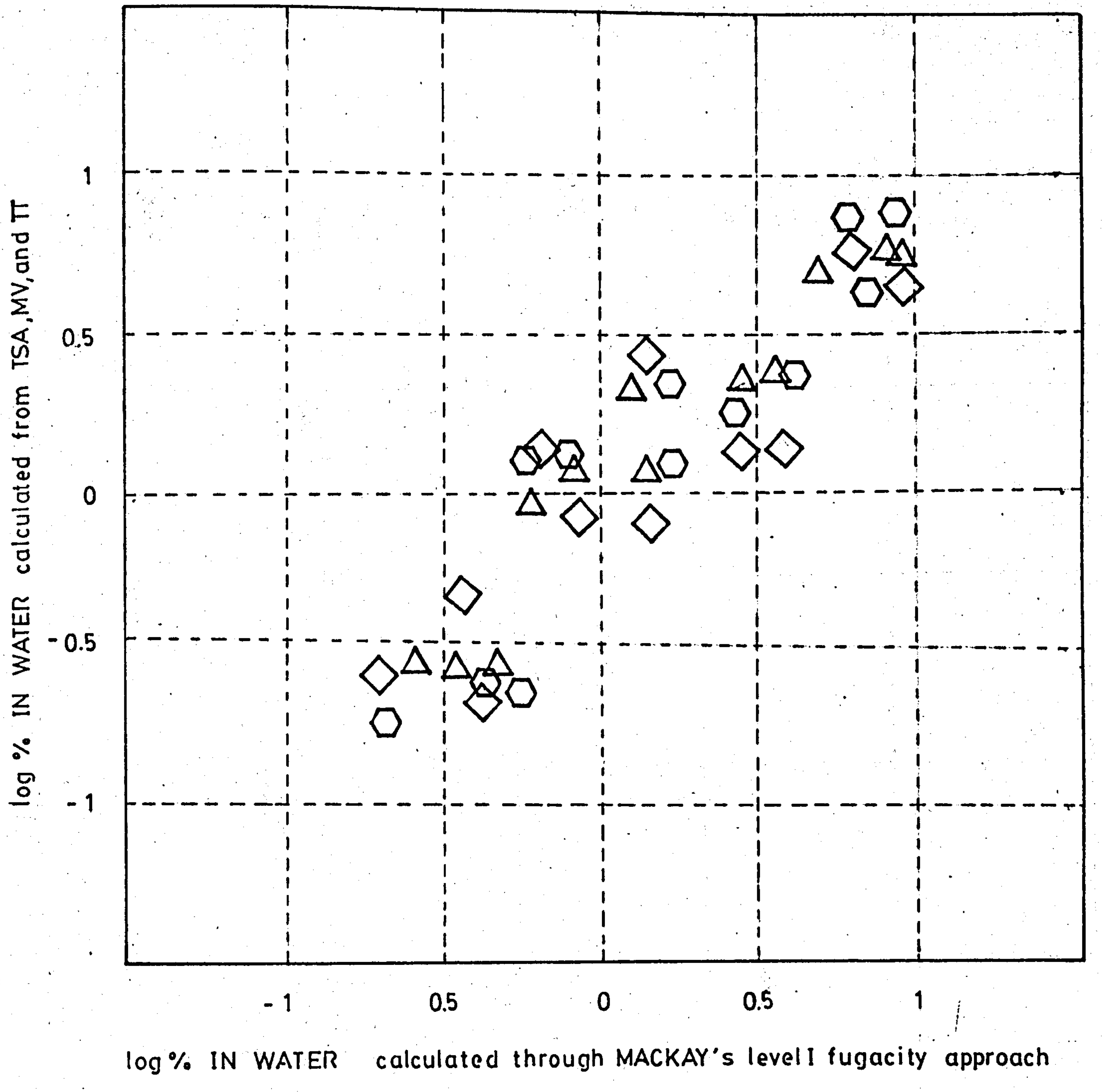


FIGURE 6.1.15 Plots of logarithm of mass partitioning into the water compartment calculated from total molecular surface area TSA by equation 58 (⬡), from molar volume MV by equation 57 (◇), from π substituent constant by equation 56 (△) versus those calculated through Mackay's level I fugacity approach for dihalogenated benzenes

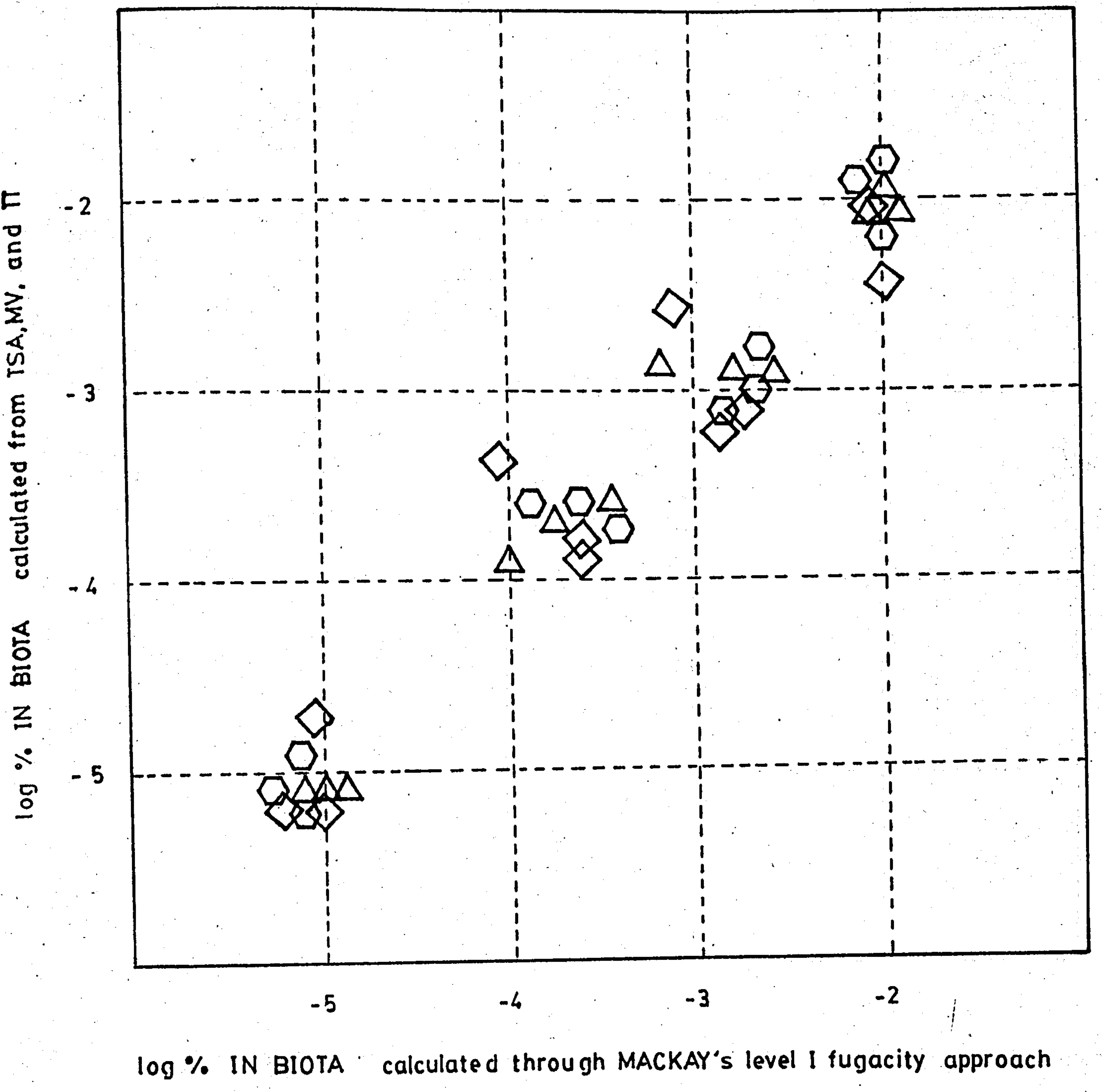


FIGURE 6.1.16. Plots of logarithm of mass partitioning into the biota compartment calculated from total molecular surface area TSA, by equation 81 (⬡), from molar volume MV by equation 80 (◇), from Π substituent constant by equation 79 (△) versus those calculated through Mackay's level I fugacity approach for dihalogenated benzenes

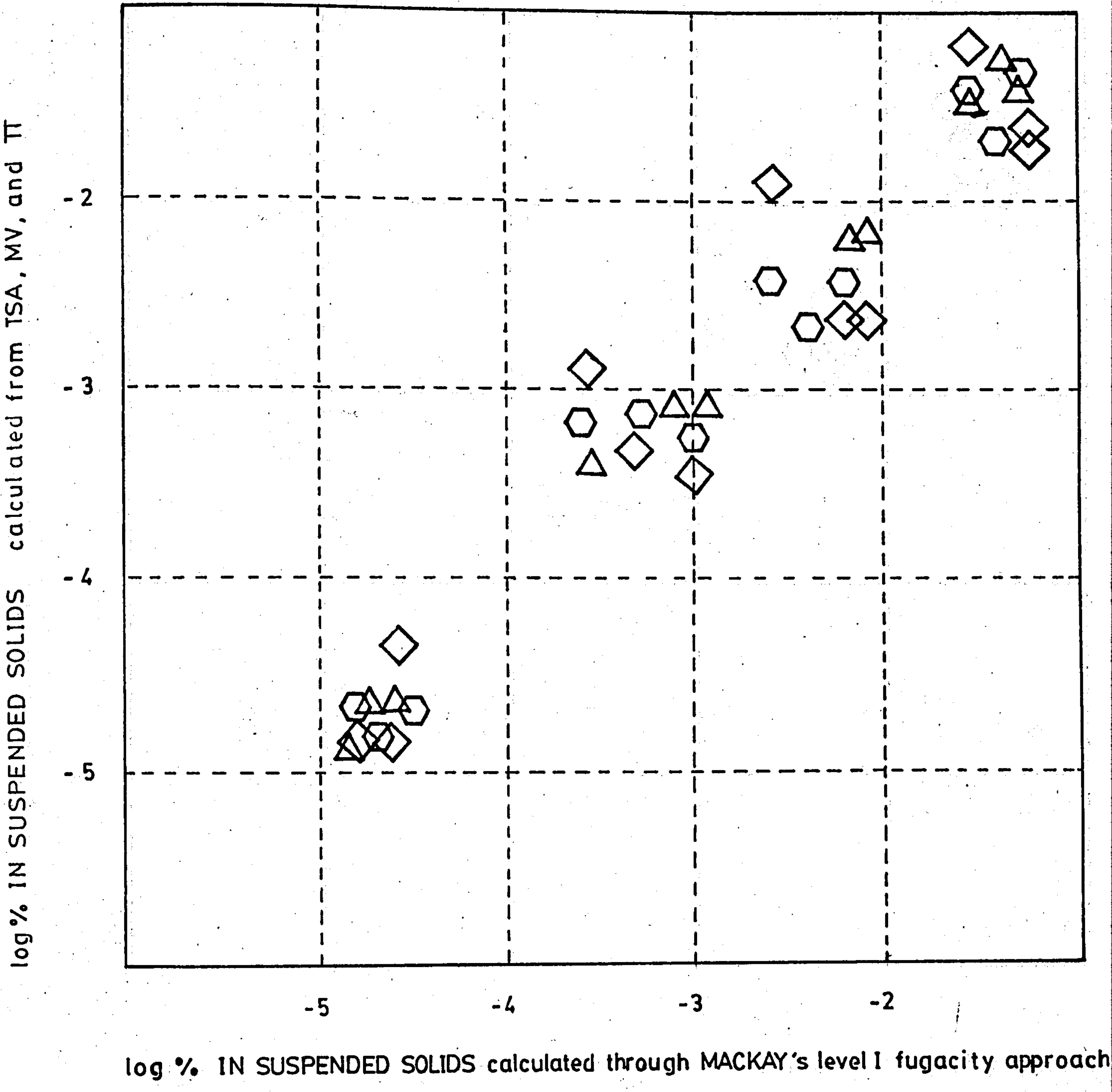


FIGURE 6.1.17 Plots of logarithm of mass partitioning into the suspended solids compartment calculated from total molecular surface area TSA by equation 104 (⬡), from molar volume MV, by equation 103 (◇), from Π substituent constant by equation 102 (△) versus those calculated through Mackay's level I fugacity approach for dihalogenated benzenes

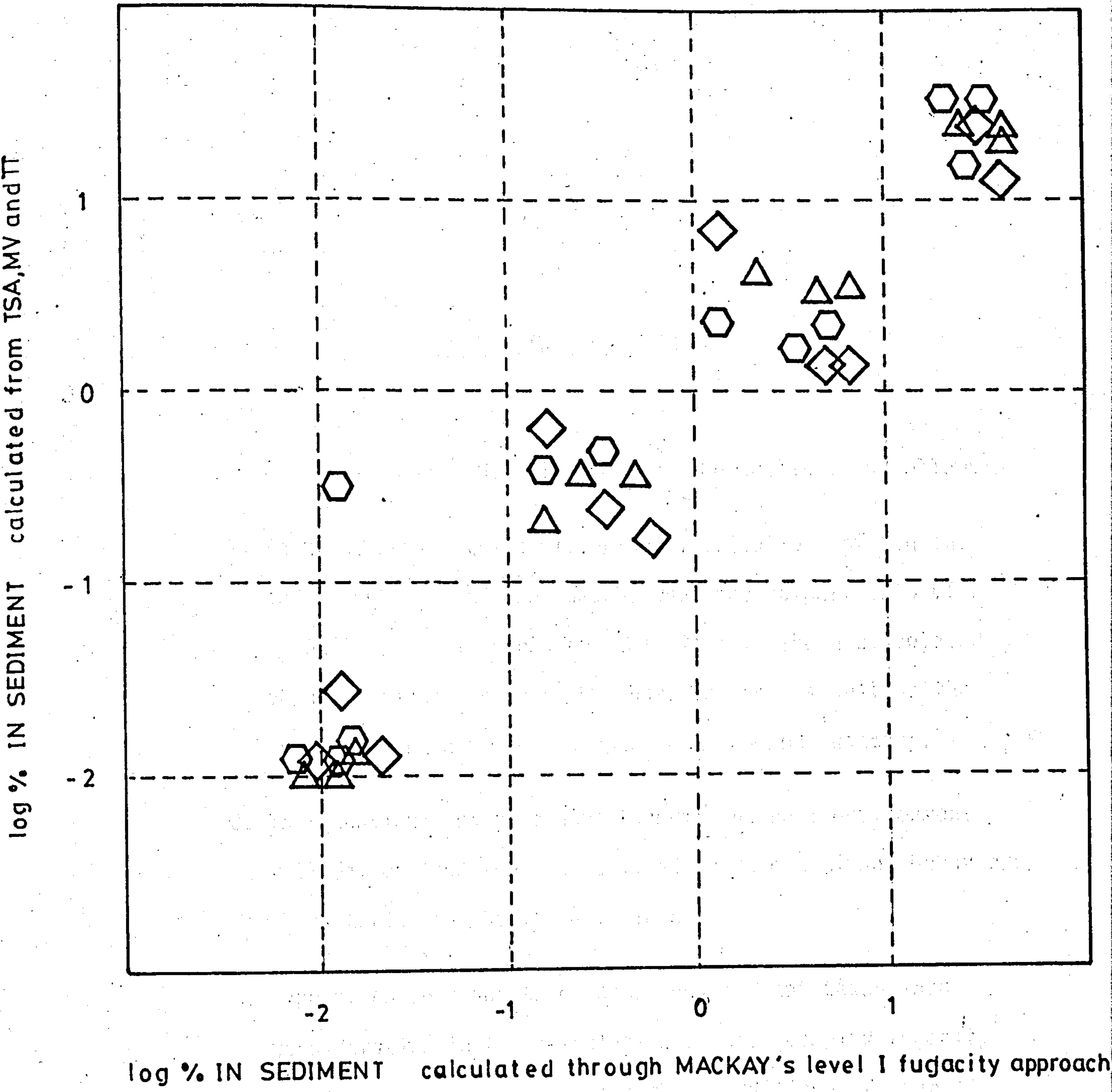


FIGURE 6.1.18. Plots of logarithm of mass partitioning into the sediment compartment calculated from total molecular surface area TSA by equation 127 (⬡), from molar volume MV, by equation 126 (◇), from π substituent constant by equation 125 (△) versus those calculated through Mackay's level I fugacity approach for dihalogenated benzenes

VII. CONCLUSIONS

Conclusions drawn from this study can be outlined as follows:

1. In this thesis, the equilibrium distributions of benzene and 72 substituted benzenes between the compartments of a hypothetical unit world are calculated. These calculated values indicate where each substance goes as well as the relative concentrations adopted at a common fugacity.

2. The behaviour and concentrations in the real environment will differ from those calculated but the dominant behaviour characteristics should be mimicked.

3. Inputs, outputs and transformations are not taken into consideration in the calculations. More complex fugacity models can be used to compare these additional features. Proceeding from level to level a profile of the environmental behaviour of the chemicals will become increasingly close to the actual environmental behaviour. On the other hand complexity will bring not only the need for more input data but also the greater possibility for errors or mistakes.

4. The calculated values are designed to set priorities for each compartment and indicate the areas in which the greatest opportunity for degradation should occur.

   a) Alkyl benzenes except butyl benzene, xylenes, mono and difluorobenzenes, mono-, di-, trichlorobenzenes, mono and dibromobenzenes, monoiodobenzene are largely dissipated into the air compartment. The potential environmental problems caused by these chemicals will be atmospheric and photodegradation becomes an area that is worthy of investigation.

   b) All phenols, all anilines, acetophenone, benzyl alcohol, butylbenzene, anisole, nitrobenzenes, diiodobenzenes, chloroiodobenzenes, bromoiodobenzenes, bromochlorobenzenes, iodobenzene, dibromobenzenes, tribromobenzenes significantly partition into water compartment therefore it is necessary to investigate whether a degradative mechanism for these compounds is available in the water compartment or not.

   c) Diiodobenzenes, tribromobenzenes, hexachlorobenzene, bromoiodobenzenes, chloroiodobenzenes, tetrachlorobenzenes, pentachlorobenzene give the expected pattern of large bioaccumulation in biota. They should be examined experimentally for degradability and also for the possibility of bioconcentration in aqueous systems.

d) Diiodobenzenes, tribromobenzenes, tetrachlorobenzenes, pentachlorobenzene, hexachlorobenzene, bromoiodobenzenes, chloroiodobenzenes significantly partition into soil, sediment, suspended solids compartments. The great affinity for soil and sediment suggests that once an aquatic ecosystem becomes contaminated, these chemicals in the sediment and soil compartments will act as a source for further contamination in the food chain long after the effects of the direct source has been terminated. The study of degradation must be conducted in these compartments.

5. If the degradation processes take place in the indicated compartments, the real amounts and concentrations will be less than expected. On the other hand, degradation products will be of concern since they adopt a new set of Z values which will partition quite differently.

6. When a group is substituted on a benzene ring, as the substituted benzenes have different physicochemical properties, they partition into different environmental compartments.

   a) The substitution of a polar group on the benzene ring such as hydroxyl or amino group cause the compound to partition mostly into the water compartment. The second group substituted on aniline and phenol does not significantly influence this partitioning.

b) The amount partitioning into the air compartment increases with the increasing number of fluorine substitution.

c) The iodine, bromine and chlorine substitution decrease the amount partitioning into the air compartment and increase the amount partitioning into the soil, sediment, suspended solids and biota compartment.

d) With the increasing number of iodine substituents, the amount partitioning into the air compartment decreases and the amounts partitioning into the soil, sediment, suspended solids and biota compartments increase significantly compared with those of the bromine substituents.

e) With the increasing number of bromine substituents the amount partitioning into the air compartment decreases and the amounts partitioning into the soil, sediment, suspended solids and biota compartments increase significantly compared with those of the chlorine substituents.

f) The substitution of nitro group on the benzene ring does not greatly influence partitioning, namely nitrobenzenes either partition into the air compartment or water compartment depending on the influence of the second substituted group on the ring.

g) Monoalkylbenzenes ultimalety partition into air compartment except butyl benzene.

h) Although monomethyl substitution causes the amount partitioning into the air compartment to increase, dimethyl substitution only causes it to decrease slightly.

7. Two physico-chemical properties namely, water solubility and vapor pressure play an important role in determining the potential impacts of chemicals in the environment. In this study it is found that the influence of vapor pressure is greater than that of solubility.

   a) Compounds having high vapor pressures ultimately partition into the air compartment even if they have high solubilities.

   b) Compounds having low vapor pressures and high solubilities mostly partition into the water compartment.

   c) Compounds having low vapor pressures, low water solubilities and thus high n-octanol-water partition coefficients partition appreciably into the biota, soil, sediment and suspended solids compartments.

It is also interesting to note that during this work good correlations between the logarithm of mass partitioning of halobenzenes and their total molecular surface area TSA, molar volume MV, and hydrophobic substituent constant π values were obtained. The mass percentage values calculated through Mackay's Level I approach were in agreement with those calculated by using the correlation equations obtained from this study. Therefore we believe these correlations will enable us to calculate the likely equilibrium distribution by using only one property TSA, MV or π.

APPENDICES

APPENDIX I

COMPUTER PROGRAMS AND OUTPUTS

A.I.I. COMPUTER PROGRAMS

THE FIRST COMPUTER PROGRAM

```
00130 REM FUGACITY CALCULATION - FUCAL
00133 REM
00135 REM
00137 REM
00138 REM
00140 REM IN THE ARRAYS,1>AIR,2>SOIL,3>WATER,4>BIOTA,5>SUS.SOLIDS,
                        6>SEDIMENT
00150 REM ARRAYS=V>VOLUME,D>DENSITY,P>ORG.CARBON PERCENT,A>AMOUNT,C>CO
        Z>FUGACITY CAPACITY CONSTANT,M>MASS PART.,E>EQUILIBRIUM PART.
00170 DIM D(6)
00180 DIM P(6)
00190 DIM Z(6)
00200 DIM M(6)
00210 DIM E(6)
00220 DIM A(6)
00230 DIM C(6)
00240 DIM T$(6)
00250 T$(1)="AIR"
00260 T$(2)="SOIL"
00270 T$(3)="WATER"
00280 T$(4)="BIOTA"
00290 T$(5)="SUSP SOLIDS"
00300 T$(6)="SEDIMENT"
00310 REM ASSIGNMENT OF VALUES TO PARAMETERS
00320 V(1)=1E+10
00330 V(2)=9E+3
00340 V(3)=7E+06
00350 V(4)=3.5
00360 V(5)=35
00370 V(6)=21000
00380 D(1)=.00119
00390 D(2)=1.5
00400 D(3)=1
00410 D(4)=1
00420 D(5)=1.5
00430 D(6)=1.5
00440 P(2)=2
00450 P(5)=4
00460 P(6)=4
00470 T=298
00480 R=8.314
00490 REM ASSIGNMENT OF VALUES TO VARIABLES
00491 REMXXXXXXXXXX  FOR K=1 TO 64
00540 INPUT C$
00560 INPUT M
00580 INPUT C8
```

Continued..

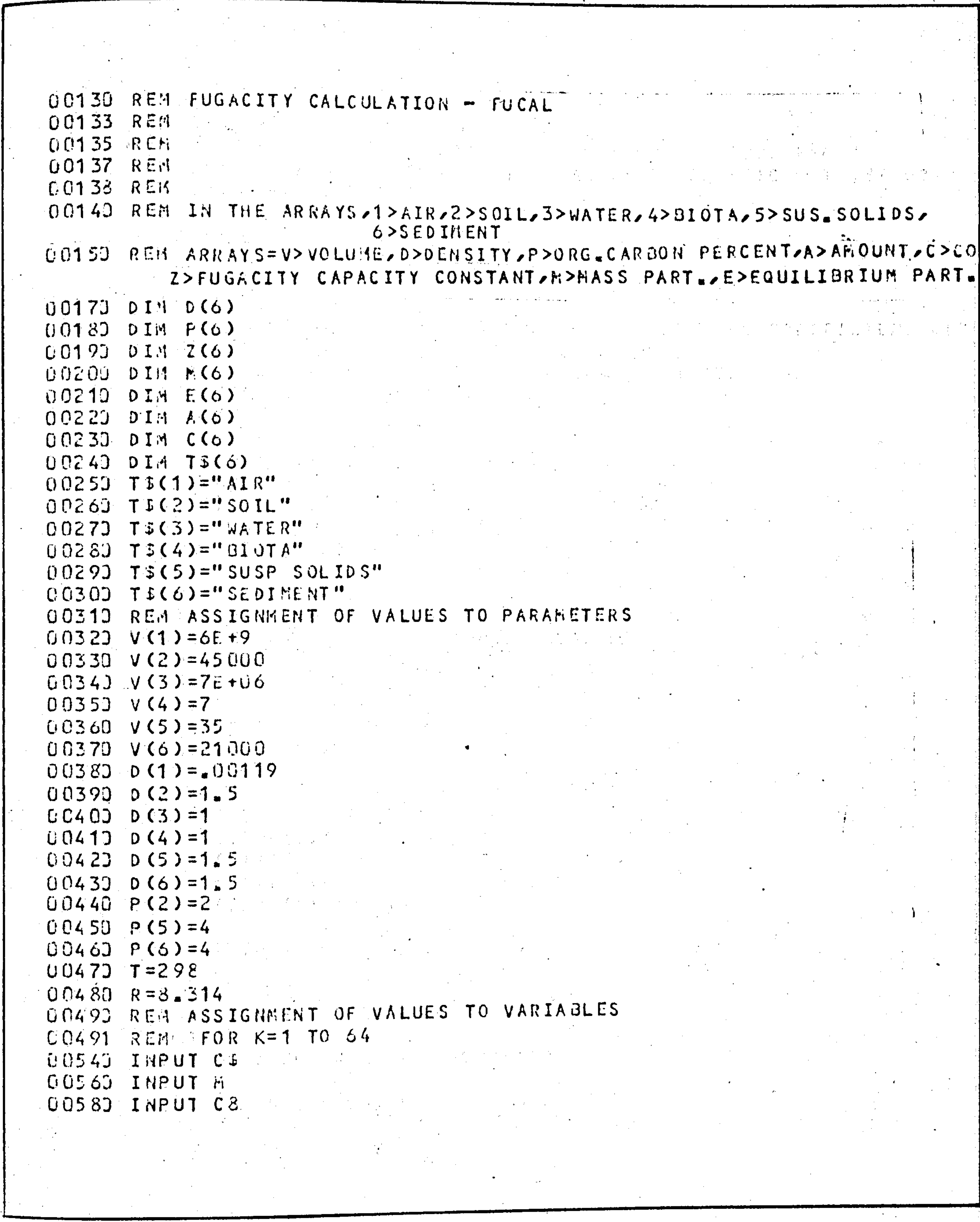
```
00600 INPUT P5
00610 P8=P5/.0075
00620 REMXXXXX PRINT "DO YOU HAVE AN EXPERIMENTAL VALUE FOR "
00630 REM XXXXX  PRINT "OCTANOL-WATER PARTITION COEFFICIENT [Y/N]? "
00640 REM XXXXX INPUT J$
00650 REM XXXXX IF J$="Y" GOTO 00690
00651 GO TO 700
00660 O8=5-.67*LOG((C8*1000)/M)/2.30259
00670 L7=O8
00680 GOTO 00710
00690 REM XXXXX PRINT "LOG OF OCTANOL-WATER PARTITION COEFFICIENT @D"
00700 INPUT L7
00710 REM CALCULATION OF FUGACITY CAPACITY CONSTANTS
00720 Z(1)=1/(R*T)
00730 H=P8*M/C8
00740 Z(3)=1/H
00750 K8=10^(.85*L7-.7)
00760 Z(4)=K8*D(4)/H
00770 K2=P(5)*.6*10^L7/100
00780 Z(5)=K2*D(5)/H
00790 K3=P(2)*.6*10^L7/100
00800 Z(2)=K3*D(2)/H
00810 K9=P(6)*.6*10^L7/100
00820 Z(6)=K9*D(6)/H
00830 REM CALCULATION OF DISTRIBUTION VALUES
00840 S8=0
00850 S5=0
00860 FOR I=1 TO 6
00870 S8=S8+Z(I)
00880 S5=S5+Z(I)*V(I)
00890 NEXT I
00900 F=100/S5
00910 FOR I=1 TO 6
00920 M(I)=Z(I)*V(I)/S5
00930 E(I)=Z(I)/S8
00940 A(I)=F*Z(I)*V(I)
00950 C(I)=A(I)/V(I)*M/D(I)
00960 NEXT I
00970 FOR I=1 TO 10
00980 PRINT
00990 NEXT I
00991 PRINT "NAME OF CHEMICAL     ";
00992 PRINT C$
00993 PRINT "MOLECULAR WEIGHT (G/MOLE)     ";
00994 PRINT M
00995 PRINT "AQEOUS SOLUBILITY (PPM)    " ;
```

Continued..

```
00997 PRINT C8
00998 PRINT "VAPOUR PRESSURE   (MM HG)";
00999 PRINT P5
 1000 PRINT "LOG OF OCTANOL-WATER PARTITION COEFFICIENT";
 1002 PRINT L7
01007 REM PRINT-OUT OF DISTRIBUTION VALUES
01010 PRINT " ","MASS PART.","EQUI.PART.","AMOUNT     ","CONCENTRATION"
01020 PRINT " ","          ","          "," (MOL)     ","   (PPM)     "
01030 PRINT
01040 FOR I=1 TO 6
01050 PRINT T$(I),M(I),E(I),A(I),C(I)
01060 PRINT
01070 NEXT I
01080 PRINT
01090 REM REPEAT PROCEDURE FOR NEW CHEMICAL
01100 REM XXXXX PRINT "'Y' TO INPUT NEW CHEMICAL...";
01110 REM XXXXX INPUT A$
01120 REM XXXXX IF A$="Y" OR A$="Y" THEN GOTO 00490
01122 REMXXXXXXXXXXX    NEXT K
01127 END
```

```
NAME OF CHEMICAL    A HYPOTHETICAL SOLUTE OF MACKAY
MOLECULAR WEIGHT (G/MOLE)    150
AQEUUS SOLUBILITY (PPM)    50
VAPOUR PRESSURE   (MM HG) .0075
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.5
                 MASS PART.     EQUI.PART.     AMOUNT         CONCENTRATION
                                               (MOL)            (PPM)

AIR              .549986        2.55472E-6     54.9986        6.93260E-4

SOIL             2.32687E-2     .120094        2.32687        2.58541E-2

WATER            .317947        2.10983E-3     31.7947        6.81315E-4

BIOTA            2.99450E-5     .397419        2.99450E-3     .128336

SUSP SOLIDS      1.80979E-4     .240188        1.80979E-2     5.17082E-2

SEDIMENT         .108587        .240188        10.8587        5.17082E-2
```

THE SECOND COMPUTER PROGRAM

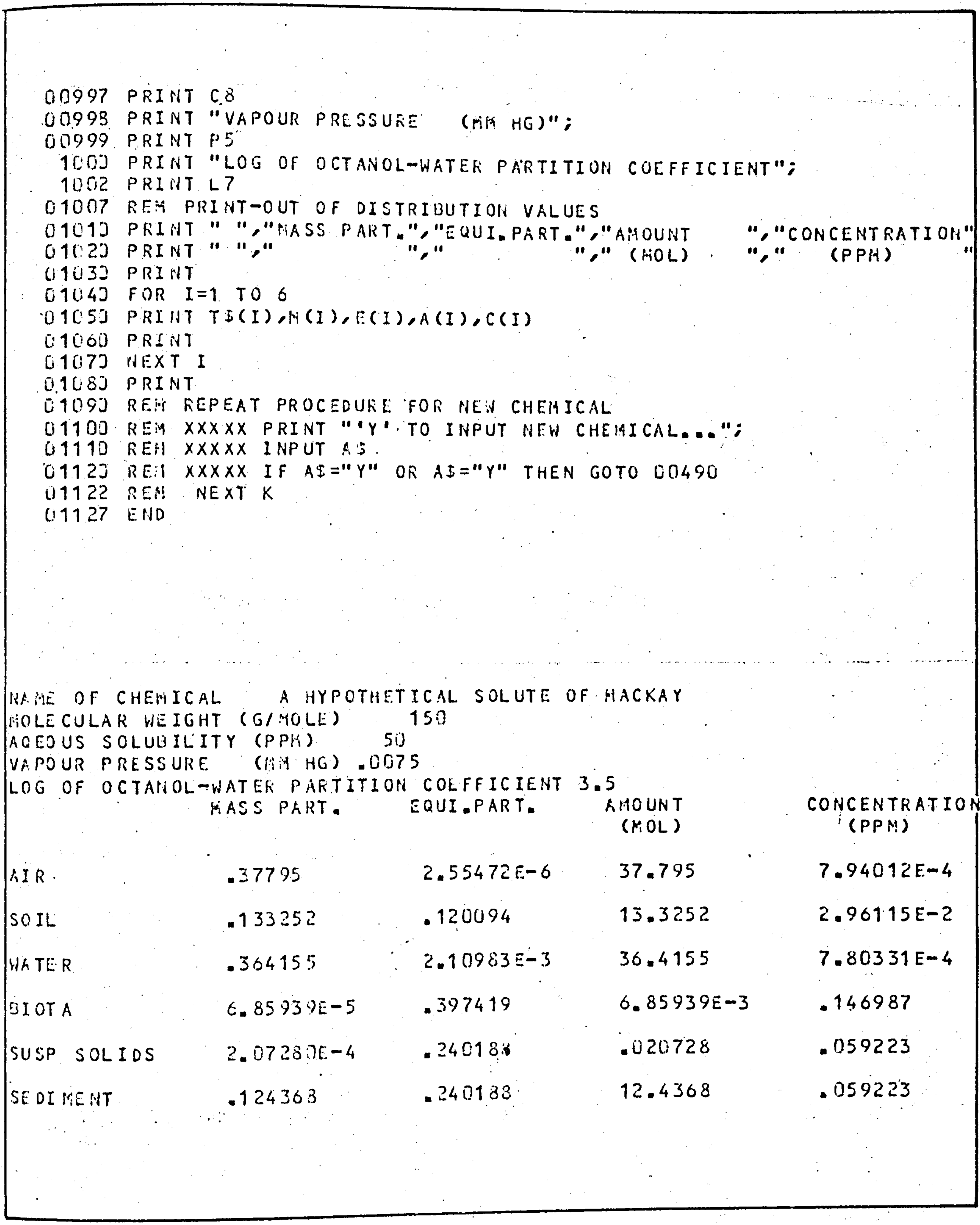


```
00130 REM FUGACITY CALCULATION - FUCAL
00133 REM
00135 REM
00137 REM
00138 REM
00140 REM IN THE ARRAYS,1>AIR,2>SOIL,3>WATER,4>BIOTA,5>SUS.SOLIDS,
                          6>SEDIMENT
00150 REM ARRAYS=V>VOLUME,D>DENSITY,P>ORG.CARBON PERCENT,A>AMOUNT,C>CO
         Z>FUGACITY CAPACITY CONSTANT,M>MASS PART.,E>EQUILIBRIUM PART.
00170 DIM D(6)
00180 DIM P(6)
00190 DIM Z(6)
00200 DIM M(6)
00210 DIM E(6)
00220 DIM A(6)
00230 DIM C(6)
00240 DIM T$(6)
00250 T$(1)="AIR"
00260 T$(2)="SOIL"
00270 T$(3)="WATER"
00280 T$(4)="BIOTA"
00290 T$(5)="SUSP SOLIDS"
00300 T$(6)="SEDIMENT"
00310 REM ASSIGNMENT OF VALUES TO PARAMETERS
00320 V(1)=6E+9
00330 V(2)=45000
00340 V(3)=7E+06
00350 V(4)=7
00360 V(5)=35
00370 V(6)=21000
00380 D(1)=.00119
00390 D(2)=1.5
00400 D(3)=1
00410 D(4)=1
00420 D(5)=1.5
00430 D(6)=1.5
00440 P(2)=2
00450 P(5)=4
00460 P(6)=4
00470 T=298
00480 R=8.314
00490 REM ASSIGNMENT OF VALUES TO VARIABLES
00491 REM  FOR K=1 TO 64
00540 INPUT C$
00560 INPUT M
00580 INPUT C8
```

Continued..

```
00600 INPUT P5
00610 P3=P5/.0075
00620 REMXXXXX PRINT "DO YOU HAVE AN EXPERIMENTAL VALUE FOR "
00630 REM XXXXX  PRINT "OCTANOL-WATER PARTITION COEFFICIENT ŞY/NO? "
00640 REM XXXXX INPUT J$
00650 REM XXXXX IF J$="Y" GOTO 00690
00651 GO TO 700
00660 08=5-.67*LOG((C8*1000)/M)/2.30259
00670 L7=08
00680 GOTO 00710
00690 REM XXXXX PRINT "LOG OF OCTANOL-WATER PARTITION COEFFICIENT ÇD"
00700 INPUT L7
00710 REM CALCULATION OF FUGACITY CAPACITY CONSTANTS
00720 Z(1)=1/(R*T)
00730 H=P3*M/C8
00740 Z(3)=1/H
00750 K8=10U(.85*L7-.7)
00760 Z(4)=K8*D(4)/H
00770 K2=P(5)*.6*10ÜL7/100
00780 Z(5)=K2*D(5)/H
00790 K3=P(2)*.6*10ÜL7/100
00800 Z(2)=K3*D(2)/H
00810 K9=P(6)*.6*10ÜL7/100
00820 Z(6)=K9*D(6)/H
00830 REM CALCULATION OF DISTRIBUTION VALUES
00840 S8=0
00850 S5=0
00860 FOR I=1 TO 6
00870 S8=S8+Z(I)
00880 S5=S5+Z(I)*V(I)
00890 NEXT I
00900 F=100/S5
00910 FOR I=1 TO 6
00920 M(I)=Z(I)*V(I)/S5
00930 E(I)=Z(I)/S8
00940 A(I)=F*Z(I)*V(I)
00950 C(I)=A(I)/V(I)*M/D(I)
00960 NEXT I
00970 FOR I=1 TO 10
00980 PRINT
00990 NEXT I
00991 PRINT "NAME OF CHEMICAL     ";
00992 PRINT C$
00993 PRINT "MOLECULAR WEIGHT (G/MOLE)     ";
00994 PRINT M
00995 PRINT "AQEOUS SOLUBILITY (PPM)     " ;
```

Continued..



```
00997 PRINT C8
00998 PRINT "VAPOUR PRESSURE   (MM HG)";
00999 PRINT P5
 1000 PRINT "LOG OF OCTANOL-WATER PARTITION COEFFICIENT";
 1002 PRINT L7
01007 REM PRINT-OUT OF DISTRIBUTION VALUES
01010 PRINT " ","MASS PART.","EQUI.PART.","AMOUNT    ","CONCENTRATION"
01020 PRINT " ","           ","           "," (MOL)    ","   (PPM)      "
01030 PRINT
01040 FOR I=1 TO 6
01050 PRINT T$(I),M(I),E(I),A(I),C(I)
01060 PRINT
01070 NEXT I
01080 PRINT
01090 REM REPEAT PROCEDURE FOR NEW CHEMICAL
01100 REM XXXXX PRINT "'Y' TO INPUT NEW CHEMICAL...";
01110 REM XXXXX INPUT A$
01120 REM XXXXX IF A$="Y" OR A$="Y" THEN GOTO 00490
01122 REM  NEXT K
01127 END
```

```
NAME OF CHEMICAL    A HYPOTHETICAL SOLUTE OF MACKAY
MOLECULAR WEIGHT (G/MOLE)     150
AQEOUS SOLUBILITY (PPM)     50
VAPOUR PRESSURE   (MM HG) .0075
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.5
                 MASS PART.     EQUI.PART.     AMOUNT         CONCENTRATION
                                               (MOL)            (PPM)

AIR               .37795         2.55472E-6     37.795         7.94012E-4

SOIL              .133252        .120094        13.3252        2.96115E-2

WATER             .364155        2.10983E-3     36.4155        7.80331E-4

BIOTA             6.85939E-5     .397419        6.85939E-3     .146987

SUSP SOLIDS       2.07280E-4     .240188        .020728        .059223

SEDIMENT          .124368        .240188        12.4368        .059223
```

A.I.2. OUTPUTS

MONOSUBSTITUTED BENZENE FAMILY

```
NAME OF CHEMICAL     BENZENE   BENZOL   C6H6
MOLECULAR WEIGHT (G/MOLE)      78.114
AQEOUS SOLUBILITY (PPM)     1790
VAPOUR PRESSURE    (MM HG) 95.044
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.13
                  MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                 (MOL)              (PPM)

AIR                .994644         8.49960E-3     99.4644          1.08817E-3

SOIL              8.11500E-5      9.24608E-2     .008115          9.39104E-6

WATER             5.19878E-3      .038079        .519878          5.80139E-6

BIOTA             6.70504E-8      .491117        6.70504E-6       7.48225E-5

SUSP SOLIDS       1.26233E-7      .184922        1.26233E-5       1.87821E-5

SEDIMENT          7.57400E-5      .184922        .007574          1.87821E-5
```

```
NAME OF CHEMICAL     FLUORO BENZENE   PHENYL FLUORIDE    C6H5.F
MOLECULAR WEIGHT (G/MOLE)      96.106
AQEOUS SOLUBILITY (PPM)     1553
VAPOUR PRESSURE    (MM HG) 77.8
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.27
                  MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                 (MOL)              (PPM)

AIR                .995336         7.41502E-3     99.5336          1.33975E-3

SOIL              9.64625E-5      9.58163E-2     9.64625E-3       1.37343E-5

WATER             4.47684E-3      2.85869E-2     .447684          6.14644E-6

BIOTA             7.59401E-8      .484917        7.59401E-6       1.04261E-4

SUSP SOLIDS       1.50053E-7      .191633        1.50053E-5       2.74685E-5

SEDIMENT          9.00316E-5      .191633        9.00316E-3       2.74685E-5
```

```
NAME OF CHEMICAL    CHLORO BENZENE   PHENYL CHLORIDE   C6H5.CL
MOLECULAR WEIGHT (G/MOLE)      112.563
AQEOUS SOLUBILITY (PPM)      480
VAPOUR PRESSURE   (MM HG) 11.6563
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.84
                     MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                   (MOL)               (PPM)

AIR                  .990923        1.27726E-3     99.0923         1.56220E-3

SOIL                 6.29140E-4     .168124        .062914         1.04915E-4

WATER                7.85887E-3     8.68262E-3     .785887         1.26374E-5

BIOTA                4.06780E-7     .449418        4.06780E-5      6.54120E-4

SUSP SOLIDS          9.78662E-7     .216249        9.78662E-5      2.09831E-4

SEDIMENT             5.87197E-4     .216249        5.87197E-2      2.09831E-4
```

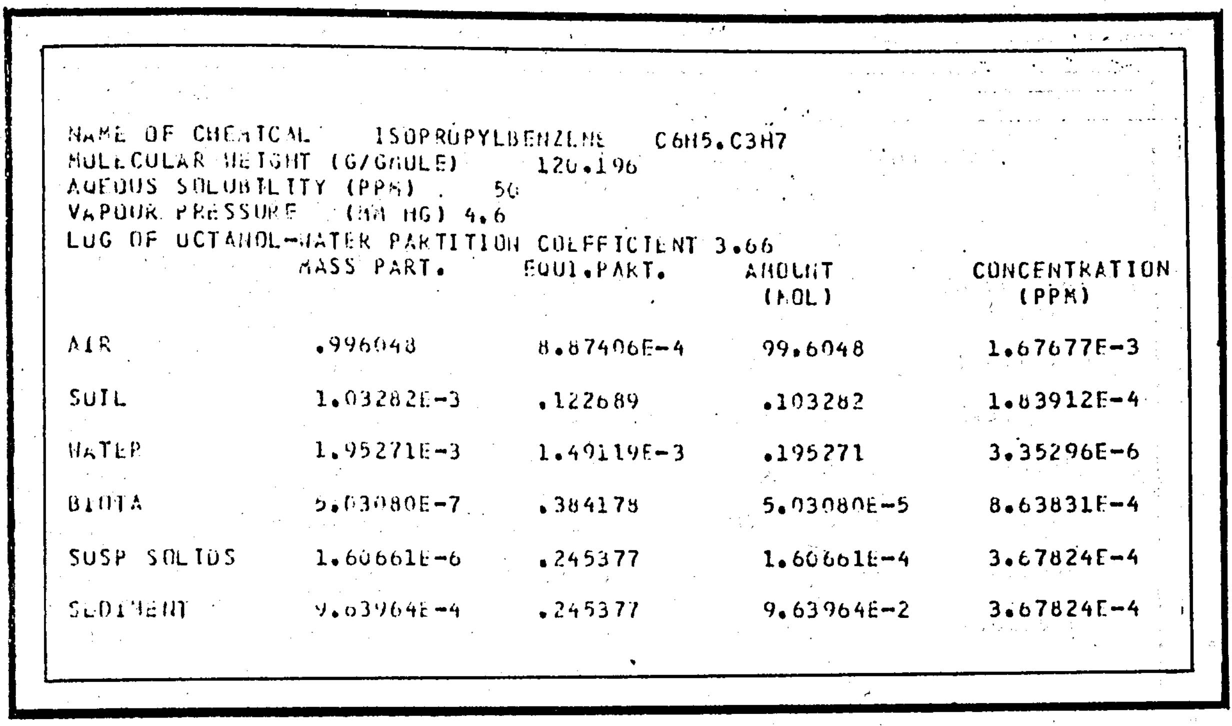
```
NAME OF CHEMICAL    BROMO BENZENE   PHENYL BROMIDE   C6H5.BR
MOLECULAR WEIGHT (G/MOLE)      157.022
AQEOUS SOLUBILITY (PPM)      410.6
VAPOUR PRESSURE   (MM HG) 4.2286
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.99
                     MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                   (MOL)               (PPM)

AIR                  .983923        5.49198E-4     98.3923         2.16383E-3

SOIL                 1.49157E-3     .111007        .149157         3.46977E-4

WATER                1.31904E-2     6.31071E-3     1.31904         2.95883E-5

BIOTA                9.15708E-7     .438105        9.15708E-5      2.05409E-3

SUSP SOLIDS          2.32022E-6     .222014        2.32022E-4      6.93954E-4

SEDIMENT             1.39213E-3     .222014        .139213         6.93954E-4
```

```
NAME OF CHEMICAL     IODOBENZENE   C6H5I
MOLECULAR WEIGHT (G/GMOLE)      204.01
AQUEOUS SOLUBILITY (PPM)      340
VAPOUR PRESSURE   (MM HG) 1.06
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.36
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                 .950958         9.76761E-5      95.0958          2.71715E-3

SOIL                8.59219E-3      .117671         .859219          2.59688E-3

WATER               3.24128E-2      2.85363E-3      3.24128          9.44649E-5

BIOTA               4.64213E-6      .408693         4.64213E-4       1.35291E-2

SUSP SOLIDS         1.33656E-5      .235342         1.33656E-3       5.19376E-3

SEDIMENT            8.01938E-3      .235342         .801938          5.19376E-3
```

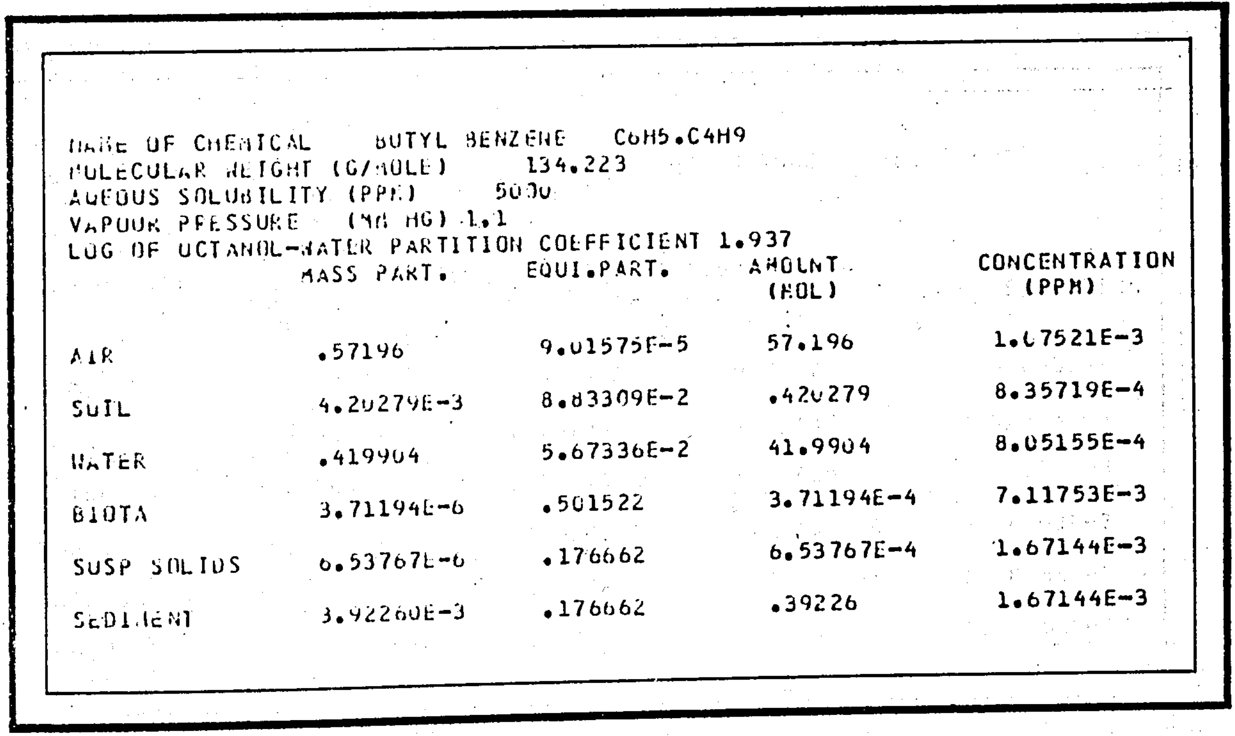
```
NAME OF CHEMICAL     METHYL BENZENE   TOLUENE   C6H5.CH3
MOLECULAR WEIGHT (G/MOLE)      92.141
AQUEOUS SOLUBILITY (PPM)      470
VAPOUR PRESSURE   (MM HG) 28.358
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.69
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                 .995691         3.56296E-3      99.5691          1.28493E-3

SOIL                2.20047E-4      .104988         2.20047E-2       3.00376E-5

WATER               3.88265E-3      1.19088E-2      .388265          5.11073E-6

BIOTA               1.49840E-7      .459587         1.49840E-5       1.97235E-4

SUSP SOLIDS         3.42295E-7      .209976         3.42295E-5       6.00751E-5

SEDIMENT            2.05377E-4      .209976         2.05377E-2       6.00751E-5
```

```
NAME OF CHEMICAL     ETHYLBENZENE    C6H5.C2H5
MOLECULAR WEIGHT (G/GMOLE)      106.169
AQUEOUS SOLUBILITY (PPM)      152
VAPOUR PRESSURE    (MM HG) 9.6
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.15
                 MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                  (MOL)              (PPM)

AIR               .995762        1.61501E-3      99.5762          1.48066E-3

SOIL              5.26201E-4     .113792         5.26201E-2       8.27648E-5

WATER             3.21932E-3     4.47547E-3      .321932          4.88275E-6

BIOTA             3.05678E-7     .424951         3.05678E-5       4.63622E-4

SUSP SOLIDS       8.18535E-7     .227584         8.18535E-5       1.65530E-4

SEDIMENT          4.91121E-4     .227584         4.91121E-2       1.65530E-4
```

```
NAME OF CHEMICAL   PROPYLBENZENE   C6H5.C3H7
MOLECULAR WEIGHT (G/GMOLE)   I20.I96
AQUEOUS SOLUBILITY (PPM)   55
VAPOUR PRESSURE    (MM HG)   3.4276
LOG OF OCTANOL -WATER PARTITION COEFFICIENT  3.68
                   MASS PART.     EQUI. PART.    AMOUNT       CONCENTRATION
                                                  (MOL)          (PPM)

AIR                .99404         5.76IE-4       99.404         I.673E-3

SOIL               I.5926E-3      0.I23          0.I5926        2.900E-4

WATER              2.8749E-3      I.428E-3       0.28749        4.936E-6

BIOTA              7.7044E-7      0.38269        7.704E-5       I.322E-3
SUSP SOLIDS        2.4775E-6      0.246I3        2.4775E-4      8.508E-4

SEDIMENT           I.4865E-3      0.246I3        0.I4865        8.508E-4
```



```
NAME OF CHEMICAL    ISOPROPYLBENZENE    C6H5.C3H7
MOLECULAR WEIGHT (G/GMOLE)       120.196
AQUEOUS SOLUBILITY (PPM)  .    50
VAPOUR PRESSURE    (MM HG) 4.6
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.66
                    MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                     (MOL)               (PPM)

AIR                  .996048        8.87406E-4      99.6048          1.67677E-3

SOIL                 1.03282E-3     .122689         .103282          1.83912E-4

WATER                1.95271E-3     1.49119E-3      .195271          3.35296E-6

BIOTA                5.03080E-7     .384178         5.03080E-5       8.63831E-4

SUSP SOLIDS          1.60661E-6     .245377         1.60661E-4       3.67824E-4

SEDIMENT             9.63964E-4     .245377         9.63964E-2       3.67824E-4
```



```
NAME OF CHEMICAL    BUTYL BENZENE    C6H5.C4H9
MOLECULAR WEIGHT (G/MOLE)       134.223
AQUEOUS SOLUBILITY (PPM)      5000
VAPOUR PRESSURE    (MM HG) 1.1
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.937
                    MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                     (MOL)               (PPM)

AIR                  .57196         9.01575E-5      57.196           1.67521E-3

SOIL                 4.20279E-3     8.83309E-2      .420279          8.35719E-4

WATER                .419904        5.67336E-2      41.9904          8.05155E-4

BIOTA                3.71194E-6     .501522         3.71194E-4       7.11753E-3

SUSP SOLIDS          6.53767E-6     .176662         6.53767E-4       1.67144E-3

SEDIMENT             3.92260E-3     .176662         .39226           1.67144E-3
```

```
NAME OF CHEMICAL
BENZYL ALCOHOL   TOLUENE α HYDROXY   PHENYL CARBINOL   C6H5.CH2OH
MOLECULAR WEIGHT (G/MOLE)       108.141
AQEOUS SOLUBILITY (PPM)      40000
VAPOUR PRESSURE    (MM HG) .0573
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.1
                    MASS PART.      EQUI.PART.      AMOUNT            CONCENTRATION
                                                     (MOL)                (PPM)

AIR                 7.07528E-3      2.16486E-6      .707528           1.07161E-5

SOIL                1.44238E-3      5.88443E-2      .144238           2.31082E-4

WATER               .990132         .259676         99.0132           1.52963E-3

BIOTA               1.70096E-6      .4461           1.70096E-4        2.62776E-3

SUSP SOLIDS         2.24370E-6      .117689         2.24370E-4        4.62165E-4

SEDIMENT            1.34622E-3      .117689         .134622           4.62165E-4
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NAME OF CHEMICAL
ACETYL BENZENE   ACETOPHENONE   METHYL PHENYL KETONE   C6H5.COCH3
MOLECULAR WEIGHT (G/MOLE)       120.152
AQEOUS SOLUBILITY (PPM)      15283
VAPOUR PRESSURE    (MM HG) .302
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.58
                    MASS PART.      EQUI.PART.      AMOUNT            CONCENTRATION
                                                     (MOL)                (PPM)

AIR                 9.79578E-2      1.44913E-5      9.79578           1.64843E-4

SOIL                3.93487E-3      7.76139E-2      .393487           7.00419E-4

WATER               .894425         .113414         89.4425           1.53524E-3

BIOTA               3.93137E-6      .498502         3.93137E-4        6.74803E-3

SUSP SOLIDS         6.12091E-6      .155228         6.12091E-4        1.40084E-3

SEDIMENT            3.67255E-3      .155228         .367255           1.40084E-3
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```
NAME OF CHEMICAL
HYDROXY BENZENE   PHENOL   CARBOLIC ACID   BENZENOL   C6H5.OH
MOLECULAR WEIGHT (G/MOLE)      94.114
AQEOUS SOLUBILITY (PPM)      93000
VAPOUR PRESSURE   (MM HG) .2948
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.46
                     MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                      (MOL)              (PPM)

AIR                  1.34887E-2      2.27054E-6      1.34887          1.77798E-5

SOIL                 3.27109E-3      7.34161E-2      .327109          4.56082E-4

WATER                .980179         .141423         98.0179          1.31784E-3

BIOTA                3.40648E-6      .491495         3.40648E-4       4.57996E-3

SUSP SOLIDS          5.08836E-6      .146832         5.08836E-4       9.12164E-4

SEDIMENT             3.05302E-3      .146832         .305302          9.12164E-4
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NAME OF CHEMICAL
METHOXY BENZENE   ANISOLE   METHYL PHENYL ETHER   C6H5.OCH3
MOLECULAR WEIGHT (G/MOLE)      108.141
AQEOUS SOLUBILITY (PPM)      10400
VAPOUR PRESSURE   (MM HG) 3.372
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.11
                     MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                      (MOL)              (PPM)

AIR                  .611199         7.54823E-5      61.1199          9.25710E-4

SOIL                 5.63326E-3      .09276          .563326          9.02498E-4

WATER                .377896         4.00026E-2      37.7896          5.83801E-4

BIOTA                4.68676E-6      .496122         4.68676E-4       7.24044E-3

SUSP SOLIDS          8.76284E-6      .18552          8.76284E-4       .001805

SEDIMENT             5.25771E-3      .18552          .525771          .001805
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NAME OF CHEMICAL     AMINO BENZENE    ANILINE    C6H5.NH2
MOLECULAR WEIGHT (G/MOLE)      93.13
AQUEOUS SOLUBILITY (PPM)      36600
VAPOUR PRESSURE    (MM HG) .4685
LOG OF OCTANOL-WATER PARTITION COEFFICIENT .9
                        MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                        (MOL)               (PPM)

AIR                     5.20359E-2      2.23039E-5      5.20359         6.78727E-5

SOIL                    8.69774E-4      4.97075E-2      8.69774E-2      1.20003E-4

WATER                   .94628          .347656         94.628          1.25896E-3

BIOTA                   1.09906E-6      .403784         1.09906E-4      1.46222E-3

SUSP SOLIDS             1.35298E-6      .099415         1.35298E-4      2.40006E-4

SEDIMENT                8.11790E-4      .099415         .081179         2.40006E-4
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NAME OF CHEMICAL
N N DIMETHYL AMINO BENZENE    N N DIMETHYL ANILINE    C6H5.N(CH3)2
MOLECULAR WEIGHT (G/MOLE)      121.184
AQUEOUS SOLUBILITY (PPM)      1254.2
VAPOUR PRESSURE    (MM HG) .741848
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.31
                        MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                        (MOL)               (PPM)

AIR                     .759721         1.02257E-4      75.9721         1.28944E-3

SOIL                    5.42853E-3      9.74221E-2      .542853         9.74594E-4

WATER                   .229771         2.65085E-2      22.9771         3.97780E-4

BIOTA                   4.21498E-6      .486279         4.21498E-4      7.29697E-3

SUSP SOLIDS             8.44438E-6      .194844         8.44438E-4      1.94919E-3

SEDIMENT                5.06663E-3      .194844         .506663         1.94919E-3
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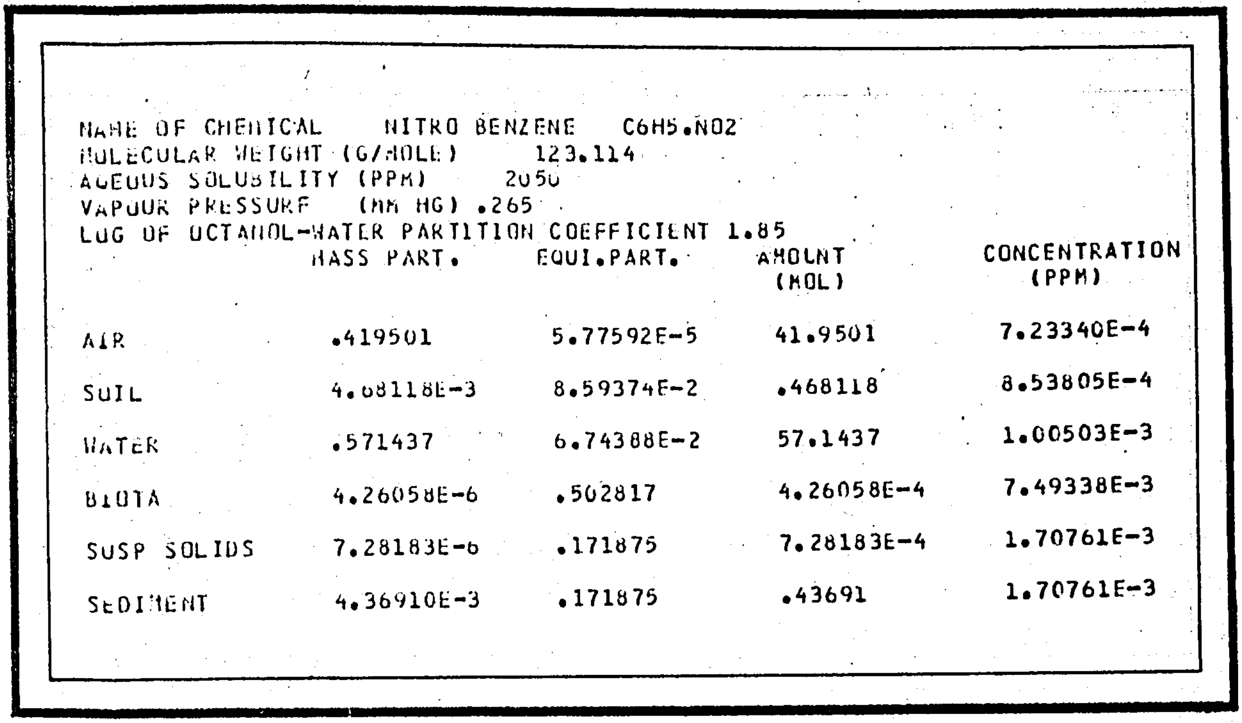

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NAME OF CHEMICAL     NITRO BENZENE   C6H5.NO2
MOLECULAR WEIGHT (G/MOLE)      123.114
AQEOUS SOLUBILITY (PPM)      2050
VAPOUR PRESSURE    (MM HG) .265
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.85
                     MASS PART.      EQUI.PART.      AMOUNT             CONCENTRATION
                                                      (MOL)                 (PPM)

AIR                   .419501         5.77592E-5      41.9501            7.23340E-4

SOIL                  4.68118E-3      8.59374E-2      .468118            8.53805E-4

WATER                 .571437         6.74388E-2      57.1437            1.00503E-3

BIOTA                 4.26058E-6      .502817         4.26058E-4         7.49338E-3

SUSP SOLIDS           7.28183E-6      .171875         7.28183E-4         1.70761E-3

SEDIMENT              4.36910E-3      .171875         .43691             1.70761E-3
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HALOBENZENE FAMILY

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NAME OF CHEMICAL     FLUORO BENZENE    PHENYL FLUORIDE   C6H5.F
MOLECULAR WEIGHT (G/MOLE)      96.106
AQUEOUS SOLUBILITY (PPM)      1553
VAPOUR PRESSURE    (MM HG) 77.8
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.27
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                    (MOL)              (PPM)

AIR                .995336         7.41502E-3      99.5336          1.33975E-3

SOIL               9.64625E-5      9.58163E-2      9.64625E-3       1.37343E-5

WATER              4.47684E-3      2.85869E-2      .447684          6.14644E-6

BIOTA              7.59401E-8      .484917         7.59401E-6       1.04261E-4

SUSP SOLIDS        1.50053E-7      .191633         1.50053E-5       2.74685E-5

SEDIMENT           9.00316E-5      .191633         9.00316E-3       2.74685E-5
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NAME OF CHEMICAL     CHLORO BENZENE    PHENYL CHLORIDE    C6H5.CL
MOLECULAR WEIGHT (G/MOLE)      112.563
AQUEOUS SOLUBILITY (PPM)      480
VAPOUR PRESSURE    (MM HG) 11.6563
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.84
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                    (MOL)              (PPM)

AIR                .990923         1.27726E-3      99.0923          1.56220E-3

SOIL               6.29140E-4      .168124         .062914          1.04915E-4

WATER              7.85887E-3      8.68262E-3      .785887          1.26374E-5

BIOTA              4.06780E-7      .449418         4.06780E-5       6.54120E-4

SUSP SOLIDS        9.76662E-7      .216249         9.76662E-5       2.09831E-4

SEDIMENT           5.87197E-4      .216249         5.87197E-2       2.09831E-4
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NAME OF CHEMICAL    BROMO BENZENE   PHENYL BROMIDE   C6H5.BR
MOLECULAR WEIGHT (G/MOLE)     157.022
AQUEOUS SOLUBILITY (PPM)     410.6
VAPOUR PRESSURE   (MM HG) 4.2286
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.99
                   MASS PART.       EQUI.PART.     AMOUNT          CONCENTRATION
                                                    (MOL)              (PPM)

AIR                .983923          5.49198E-4     98.3923          2.16383E-3

SOIL               1.49157E-3       .111607        .149157          3.46977E-4

WATER              1.31904E-2       6.31071E-3     1.31904          2.95883E-5

BIOTA              9.15708E-7       .438105        9.15708E-5       2.05409E-3

SUSP SOLIDS        2.32022E-6       .222014        2.32022E-4       6.93954E-4

SEDIMENT           1.39213E-3       .222014        .139213          6.93954E-4
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NAME OF CHEMICAL    IODOBENZENE    C6H5I
MOLECULAR WEIGHT (G/MOLE)     204.01
AQUEOUS SOLUBILITY (PPM)     340
VAPOUR PRESSURE   (MM HG) 1.00
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.36
                   MASS PART.       EQUI.PART.     AMOUNT          CONCENTRATION
                                                    (MOL)              (PPM)

AIR                .950958          9.76761E-5     95.0958          2.71715E-3

SOIL               6.59219E-3       .117671        .659219          2.59088E-3

WATER              3.24128E-2       2.85363E-3     3.24128          9.44649E-5

BIOTA              4.64213E-6       .406093        4.64213E-4       1.35291E-2

SUSP SOLIDS        1.33656E-5       .235342        1.33656E-3       5.19376E-3

SEDIMENT           8.01938E-3       .235342        .801938          5.19376E-3
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NAME OF CHEMICAL     O DIFLUOROBENZENE
MOLECULAR WEIGHT (G/GMOLE)     114.09
AQEOUS SOLUBILITY (PPM)     1140.9
VAPOUR PRESSURE   (MM HG) 62.5957
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.59
                     MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                      (MOL)              (PPM)

AIR                  .996249          4.94786E-3      99.6249         1.59191E-3

SOIL                 1.55326E-4       .102857         1.55326E-2      2.62536E-5

WATER                3.45031E-3       1.46879E-2      .345031         5.62351E-6

BIOTA                1.09486E-7       .46608          1.09486E-5      1.78446E-4

SUSP SOLIDS          2.41619E-7       .205714         2.41619E-5      5.25072E-5

SEDIMENT             1.44971E-4       .205714         1.44971E-2      5.25072E-5
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NAME OF CHEMICAL     M DIFLUOROBENZENE
MOLECULAR WEIGHT (G/GMOLE)     114.09
AQEOUS SOLUBILITY (PPM)     1140.9
VAPOUR PRESSURE   (MM HG) 89.663
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.58
                     MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                      (MOL)              (PPM)

AIR                  .997383          7.22172E-3      99.7383         1.59372E-3

SOIL                 1.06089E-4       .102421         1.06089E-2      1.79314E-5

WATER                2.41148E-3       1.49663E-2      .241148         3.93036E-6

BIOTA                7.50383E-8       .465709         7.50383E-6      1.22302E-4

SUSP SOLIDS          1.65027E-7       .204841         1.65027E-5      3.58628E-5

SEDIMENT             9.90163E-5       .204841         9.90163E-3      3.58628E-5
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NAME OF CHEMICAL     P DIFLUOROBENZENE
MOLECULAR WEIGHT (G/GMOLE)      114.09
AQEOUS SOLUBILITY (PPM)      1224.4
VAPOUR PRESSURE    (MM HG) 70.614
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.58
                    MASS PART.       EQUI.PART.       AMOUNT            CONCENTRATION
                                                      (MOL)                (PPM)

AIR                  .996437         5.30980E-3       99.6437           1.59221E-3

SOIL                 1.44430E-4      .102618          .014443           2.44118E-5

WATER                3.28299E-3      1.49951E-2       .328299           5.35080E-6

BIOTA                1.02157E-7      .466606          1.02157E-5        1.66502E-4

SUSP SOLIDS          2.24668E-7      .205236          2.24668E-5        4.88236E-5

SEDIMENT             1.34801E-4      .205236          1.34801E-2        4.88236E-5
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NAME OF CHEMICAL      O DICHLOROBENZENE    C6H4CL2
MOLECULAR WEIGHT (G/GMOLE)       147.01
AQEOUS SOLUBILITY (PPM)       150
VAPOUR PRESSURE    (MM HG) 1.392
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.59
                    MASS PART.       EQUI.PART.       AMOUNT            CONCENTRATION
                                                      (MOL)                (PPM)

AIR                  .971123         1.27494E-4       97.1123           1.99951E-3

SOIL                 6.94705E-3      .121606          .694705           1.51302E-3

WATER                1.54317E-2      1.73653E-3       1.54317           3.24088E-5

BIOTA                3.46668E-6      .390106          3.46668E-4        7.28052E-3

SUSP SOLIDS          1.08065E-5      .243212          1.08065E-3        3.02603E-3

SEDIMENT             6.48392E-3      .243212          .648392           3.02603E-3
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NAME OF CHEMICAL     M DICHLOROBENZENE   147.01
MOLECULAR WEIGHT (G/GMOLE)      147.01
AQEOUS SOLUBILITY (PPM)       120
VAPOUR PRESSURE    (MM HG) 2.243
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.59
                          MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                           (MOL)               (PPM)

AIR                       .985452         2.56764E-4      98.5452           2.02901E-3

SOIL                      3.49995E-3      .12159          .349995           7.62263E-4

WATER                     7.77454E-3      1.73631E-3      .777454           1.63276E-5

BIOTA                     1.74652E-6      .390655         1.74652E-4        3.66795E-3

SUSP SOLIDS               5.44437E-6      .243181         5.44437E-4        1.52453E-3

SEDIMENT                  3.26662E-3      .243181         .326662           1.52453E-3
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NAME OF CHEMICAL     P DICHLOR BENZENE    C6H4.CL2
MOLECULAR WEIGHT (G/MOLE)       147.012
AQEUUS SOLUBILITY (PPM)       79
VAPOUR PRESSURE    (MM HG) 1.926
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.38
                          MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                           (MOL)               (PPM)

AIR                       .990788         5.26969E-4      99.0788           2.04002E-3

SOIL                      1.66349E-3      .117968         .166349           3.62300E-4

WATER                     5.99284E-3      2.73206E-3      .599284           1.25860E-5

BIOTA                     8.92551E-7      .406903         8.92551E-5        1.87451E-3

SUSP SOLIDS               2.58765E-6      .235935         2.58765E-4        7.24601E-4

SEDIMENT                  1.55259E-3      .235935         .155259           7.24601E-4
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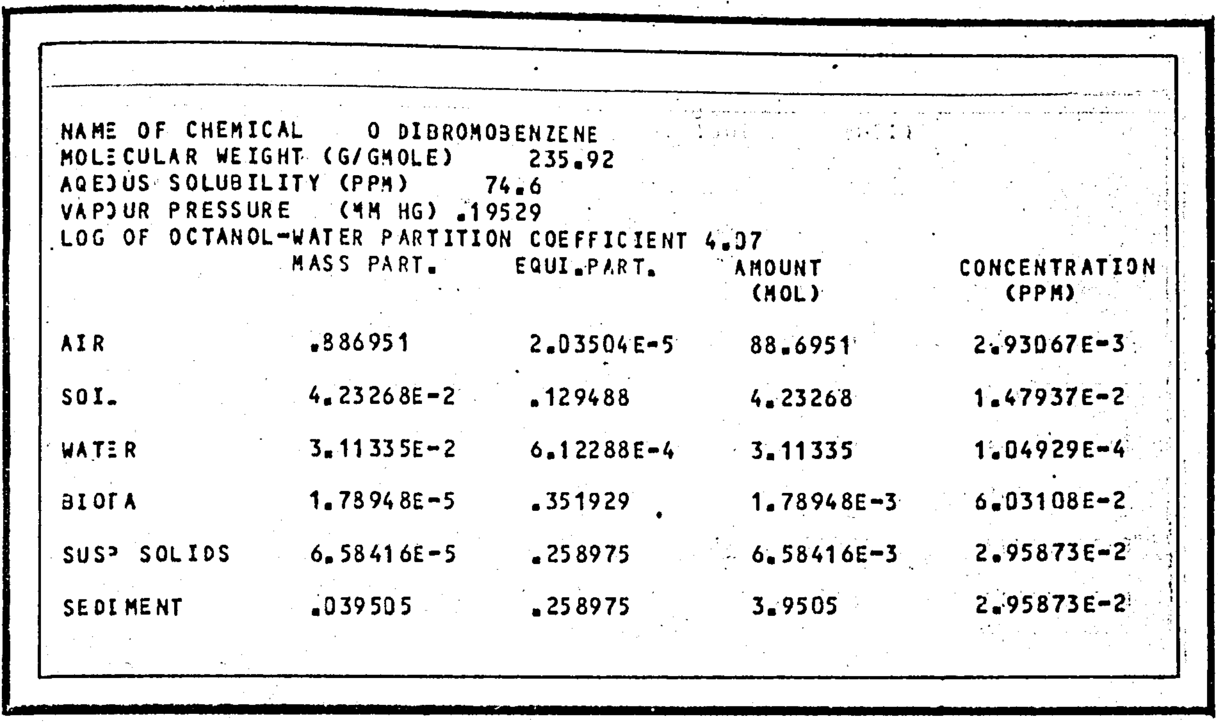

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NAME OF CHEMICAL     O DIBROMOBENZENE
MOLECULAR WEIGHT (G/GMOLE)     235.92
AQEOUS SOLUBILITY (PPM)     74.6
VAPOUR PRESSURE   (MM HG) .19529
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.07
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                  .886951         2.03504E-5      88.6951          2.93067E-3

SOIL                 4.23268E-2      .129488         4.23268          1.47937E-2

WATER                3.11335E-2      6.12288E-4      3.11335          1.04929E-4

BIOTA                1.78948E-5      .351929         1.78948E-3       6.03108E-2

SUSP SOLIDS          6.58416E-5      .258975         6.58416E-3       2.95873E-2

SEDIMENT             .039505         .258975         3.9505           2.95873E-2
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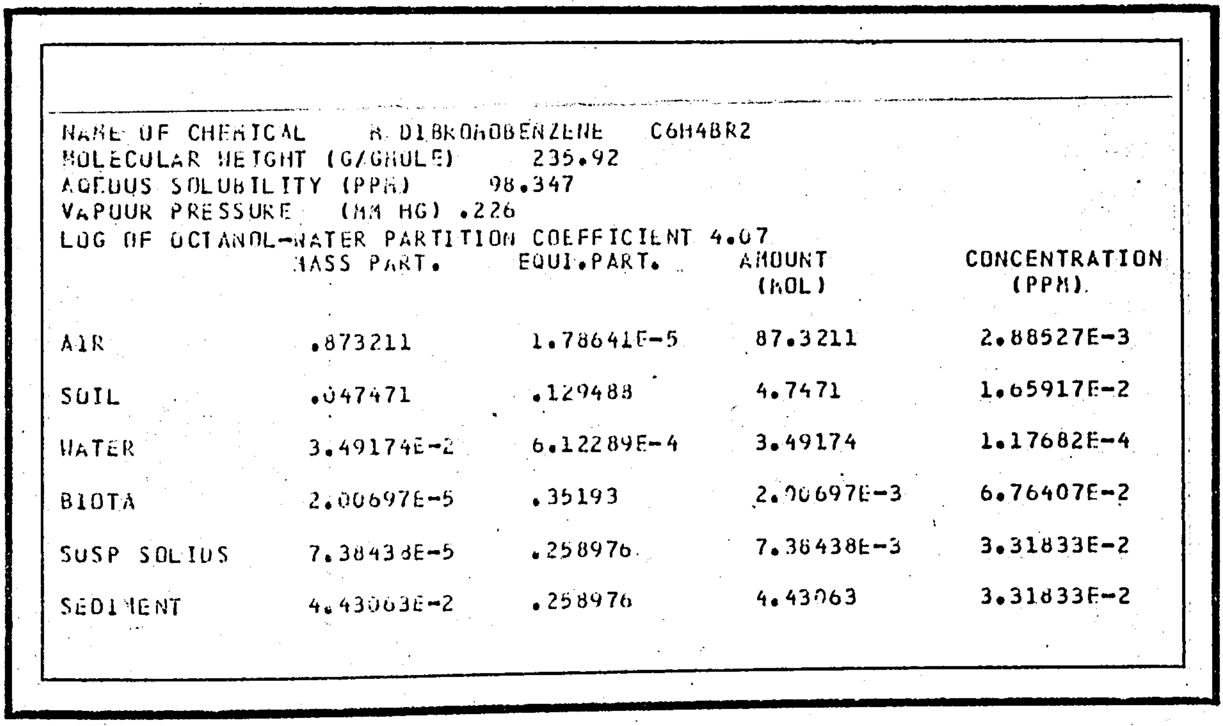

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NAME OF CHEMICAL     M DIBROMOBENZENE    C6H4BR2
MOLECULAR WEIGHT (G/GMOLE)     235.92
AQEOUS SOLUBILITY (PPM)     98.347
VAPOUR PRESSURE   (MM HG) .226
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.07
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                  .873211         1.78641E-5      87.3211          2.88527E-3

SOIL                 .047471         .129488         4.7471           1.65917E-2

WATER                3.49174E-2      6.12289E-4      3.49174          1.17682E-4

BIOTA                2.00697E-5      .35193          2.00697E-3       6.76407E-2

SUSP SOLIDS          7.38438E-5      .258976         7.38438E-3       3.31833E-2

SEDIMENT             4.43063E-2      .258976         4.43063          3.31833E-2
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NAME OF CHEMICAL     P DIBROMOBENZENE
MOLECULAR WEIGHT (G/GMOLE)       235.92
AQEOUS SOLUBILITY (PPM)      20.08
VAPOUR PRESSURE    (MM HG) .16112
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.07
                   MASS PART.      EQUI.PART.       AMOUNT          CONCENTRATION
                                                     (MOL)               (PPM)

AIR                .960077          6.23735E-5       96.0077          3.17229E-3

SOIL               1.49478E-2       .129482          1.49478          5.22441E-3

WATER              1.09949E-2       6.12262E-4       1.09949          3.70558E-5

BIOTA              6.31960E-6       .351915          6.31960E-4       2.12989E-2

SUSP SOLIDS        2.32521E-5       .258964          2.32521E-3       1.04488E-2

SEDIMENT           1.39513E-2       .258964          1.39513          1.04488E-2
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NAME OF CHEMICAL     O DIIODOBENZENE
MOLECULAR WEIGHT (G/GMOLE)       329.91
AQEOUS SOLUBILITY (PPM)      18.9843
VAPOUR PRESSURE    (MM HG) .007258
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.65
                   MASS PART.      EQUI.PART.       AMOUNT          CONCENTRATION
                                                     (MOL)               (PPM)

AIR                .345887          1.16836E-6       34.5887          1.59820E-3

SOIL               .307282          .138394          30.7282          .150186

WATER              5.94498E-2       1.72126E-4       5.94498          2.80187E-4

BIOTA              1.06329E-4       .307855          1.06329E-2       .501127

SUSP SOLIDS        4.77995E-4       .276789          4.77995E-2       .300372

SEDIMENT           .286797          .276789          28.6797          .300372
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NAME OF CHEMICAL     M DIIODOBENZENE
MOLECULAR WEIGHT (G/GMOLE)      329.91
AQEOUS SOLUBILITY (PPM)      8.8796
VAPOUR PRESSURE    (MM HG) .00568
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.64
                  MASS PART.      EQUI.PART.     AMOUNT          CONCENTRATION
                                                 (MOL)              (PPM)

AIR                .474633         1.99822E-6     47.4633          2.19308E-3

SOIL               .24628          .138246        24.628           .120371

WATER              4.87575E-2      1.75947E-4     4.87575          2.29794E-4

BIOTA              8.55149E-5      .30859         8.55149E-3       .403032

SUSP SOLIDS        3.83102E-4      .276493        3.83102E-2       .240741

SEDIMENT           .229861         .276493        22.9861          .240741
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NAME OF CHEMICAL     P DIIODOBENZENE
MOLECULAR WEIGHT (G/GMOLE)      329.91
AQEOUS SOLUBILITY (PPM)      1.855
VAPOUR PRESSURE    (MM HG) 6.96800E-4
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.64
                  MASS PART.      EQUI.PART.     AMOUNT          CONCENTRATION
                                                 (MOL)              (PPM)

AIR                .346629         1.17342E-6     34.6629          1.60163E-3

SOIL               .306285         .138247        30.6285          .149699

WATER              6.06372E-2      1.75947E-4     6.06372          2.85783E-4

BIOTA              1.06350E-4      .30859         .010635          .501229

SUSP SOLIDS        4.76444E-4      .276493        4.76444E-2       .299397

SEDIMENT           .285866         .276493        28.5866          .299397
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NAME OF CHEMICAL     O BROMOCHLOROBENZENE
MOLECULAR WEIGHT (G/GMOLE)     191.46
AQEOUS SOLUBILITY (PPM)     123.617
VAPOUR PRESSURE   (MM HG) .44249
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.83
                    MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR                 .926333        3.80681E-5     92.6333         2.48397E-3

SOIL                2.29237E-2     .125608        2.29237         6.50218E-3

WATER               .029302        1.03215E-3     2.9302          8.01452E-5

BIOTA               1.05293E-5     .37089         1.05293E-3      .028799

SUSP SOLIDS         3.56591E-5     .251216        3.56591E-3      1.30044E-2

SEDIMENT            2.13954E-2     .251216        2.13954         1.30044E-2
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NAME OF CHEMICAL     M BROMOCHLOROBENZENE
MOLECULAR WEIGHT (G/GMOLE)     191.46
AQEOUS SOLUBILITY (PPM)     118.053
VAPOUR PRESSURE   (MM HG) .64645
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.83
                    MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR                 .950584        5.82350E-5     95.0584         .002549

SOIL                1.53772E-2     .125605        1.53772         4.36165E-3

WATER               1.96558E-2     1.03213E-3     1.96558         5.37613E-5

BIOTA               7.06301E-6     .370882        7.06301E-4      1.93183E-2

SUSP SOLIDS         2.39201E-5     .251211        2.39201E-3      8.72330E-3

SEDIMENT            .014352        .251211        1.4352          8.72330E-3
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```
NAME OF CHEMICAL     P BROMOCHLOROBENZENE   C6H4BRCL
MOLECULAR WEIGHT (G/GMOLE)       191.46
AQUEOUS SOLUBILITY (PPM)      44.882
VAPOUR PRESSURE   (MM HG) .63313
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 3.83
                    MASS PART.      EQUI.PART.       AMOUNT           CONCENTRATION
                                                      (MOL)               (PPM)

AIR                 .98022          1.50006E-4       98.022            2.62847E-3

SOIL                6.15525E-3      .125594          .615525           1.74590E-3

WATER               7.86790E-3      1.03204E-3       .78679            2.15198E-5

BIOTA               2.82722E-6      .370848          2.82722E-4        7.73284E-3

SUSP SOLIDS         9.57484E-6      .251188          9.57484E-4        3.49181E-3

SEDIMENT            5.74490E-3      .251188          .57449            3.49181E-3
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```
NAME OF CHEMICAL     P BROMOIODOBENZENE    C6H4BRI
MOLECULAR WEIGHT (G/GMOLE)       282.91
AQUEOUS SOLUBILITY (PPM)      7.79
VAPOUR PRESSURE    (MM HG) .00923
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.36
                    MASS PART.      EQUI.PART.       AMOUNT           CONCENTRATION
                                                      (MOL)               (PPM)

AIR                 .7161           5.86325E-6       71.61             2.83742E-3

SOIL                .122767         .134025          12.2767           5.14549E-2

WATER               4.63122E-2      3.25022E-4       4.63122           1.87174E-4

BIOTA               4.69565E-5      .329544          4.69565E-3        .189778

SUSP SOLIDS         1.90971E-4      .26805           1.90971E-2        .10291

SEDIMENT            .114583         .26805           11.4583           .10291
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```
NAME OF CHEMICAL    O CHLOROIODOBENZENE   C6H4ICL
MOLECULAR WEIGHT (G/GMOLE)      236.46
AQEOUS SOLUBILITY (PPM)      68.77
VAPOUR PRESSURE   (MM HG) .1012
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.12
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR               .803757         1.03687E-5      80.3757           2.68437E-3

SOIL              7.57442E-2      .130283         7.57442           2.67584E-2

WATER             4.96549E-2      5.49052E-4      4.96549           1.69153E-4

BIOTA             3.14747E-5      .348028         3.14747E-3        .107221

SUSP SOLIDS       1.17824E-4      .260565         1.17824E-2        5.35169E-2

SEDIMENT          7.06945E-2      .260565         7.06945           5.35169E-2
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```
NAME OF CHEMICAL    M CHLOROIODOBENZENE   C6H4ICL
MOLECULAR WEIGHT (G/GMOLE).     238.46
AQEOUS SOLUBILITY (PPM)      67.207
VAPOUR PRESSURE   (MM HG) .126
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.12
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR               .839177         1.32098E-5      83.9177           2.80266E-3

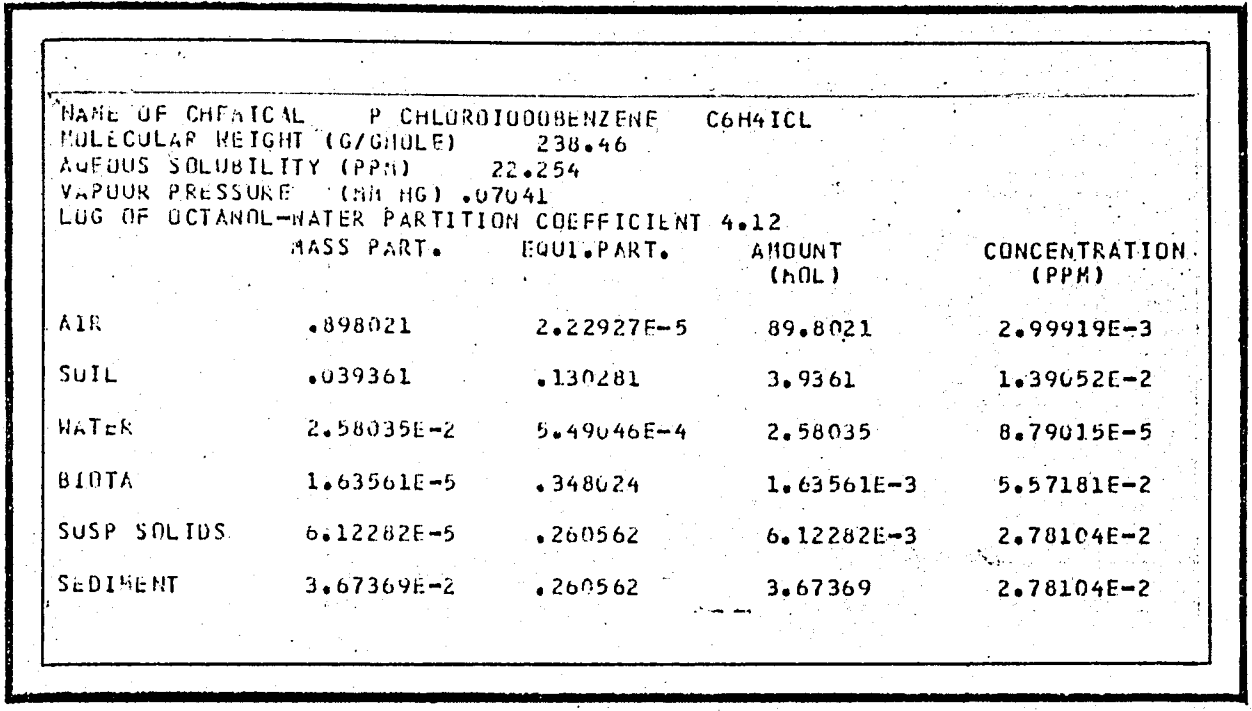
SOIL              6.20731E-2      .130282         6.20731           2.19288E-2

WATER             4.06927E-2      5.49051E-4      4.06927           1.38623E-4

BIOTA             2.57939E-5      .348027         2.57939E-3        8.78686E-2

SUSP SOLIDS       9.65581E-5      .260564         9.65581E-3        4.38576E-2

SEDIMENT          5.79349E-2      .260564         5.79349           4.38576E-2
```



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NAME OF CHEMICAL     P CHLOROIODOBENZENE    C6H4ICL
MOLECULAR WEIGHT (G/GMOLE)        238.46
AQEOUS SOLUBILITY (PPM)       22.254
VAPOUR PRESSURE    (MM HG) .07041
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.12
                   MASS PART.     EQUI.PART.      AMOUNT            CONCENTRATION
                                                   (MOL)                (PPM)

AIR                .898021         2.22927E-5      89.8021            2.99919E-3

SOIL               .039361         .130281         3.9361             1.39052E-2

WATER              2.58035E-2      5.49046E-4      2.58035            8.79015E-5

BIOTA              1.63561E-5      .348024         1.63561E-3         5.57181E-2

SUSP SOLIDS        6.12282E-5      .260562         6.12282E-3         2.78104E-2

SEDIMENT           3.67369E-2      .260562         3.67369            2.78104E-2
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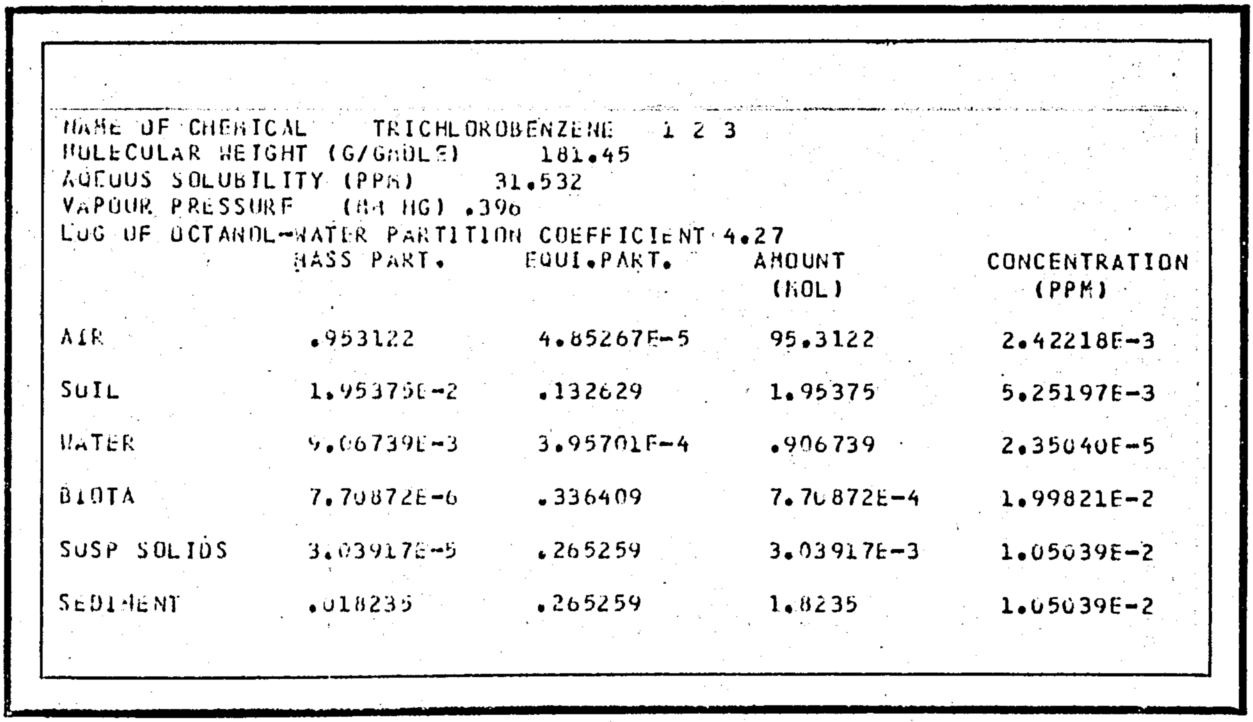

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NAME OF CHEMICAL      TRICHLOROBENZENE    1 2 3
MOLECULAR WEIGHT (G/GMOLE)        181.45
AQEOUS SOLUBILITY (PPM)       31.532
VAPOUR PRESSURE    (MM HG) .396
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.27
                   MASS PART.     EQUI.PART.      AMOUNT            CONCENTRATION
                                                   (MOL)                (PPM)

AIR                .953122         4.85267E-5      95.3122            2.42218E-3

SOIL               1.95375E-2      .132629         1.95375            5.25197E-3

WATER              9.06739E-3      3.95701E-4      .906739            2.35040E-5

BIOTA              7.70872E-6      .336409         7.70872E-4         1.99821E-2

SUSP SOLIDS        3.03917E-5      .265259         3.03917E-3         1.05039E-2

SEDIMENT           .018235         .265259         1.8235             1.05039E-2
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NAME OF CHEMICAL     TRICHLOR BENZENE 1 2 4    C6H3.CL3
MOLECULAR WEIGHT (G/MOLE)       181.461
AQUEOUS SOLUBILITY (PPM)      30
VAPOUR PRESSURE    (MM HG) .426512
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.176
                   MASS PART.      EQUI.PART.       AMOUNT          CONCENTRATION
                                                    (MOL)               (PPM)

AIR                 .96467          6.74573E-5       96.467          2.45168E-3

SOIL                1.40672E-2      .131158          1.40672         3.78169E-3

WATER               8.10624E-3      4.85873E-4       .810624         2.10138E-5

BIOTA               5.73350E-6      .343655          5.73350E-4      1.48629E-2

SUSP SOLIDS         2.18823E-5      .262317          2.18823E-3      7.56338E-3

SEDIMENT            1.31294E-2      .262317          1.31294         7.56338E-3
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NAME OF CHEMICAL      TRICHLOROBENZENE    1 3 5
MOLECULAR WEIGHT (G/GMOLE)        181.45
AQUEOUS SOLUBILITY (PPM)       6.588
VAPOUR PRESSURE    (MM HG) .8363
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.27
                   MASS PART.      EQUI.PART.       AMOUNT          CONCENTRATION
                                                    (MOL)               (PPM)

AIR                 .995158         4.90290E-4       99.5158         2.52901E-3

SOIL                2.01812E-3      .132571          .201812         5.42502E-4

WATER               9.36614E-4      3.95526E-4       9.36614E-2      2.42784E-6

BIOTA               7.96271E-7      .33626           7.96271E-5      2.06405E-3

SUSP SOLIDS         3.13930E-6      .265142          3.13930E-4      .001085

SEDIMENT            1.88358E-3      .265142          .188358         .001085
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```
NAME OF CHEMICAL     TRIBROMOBENZENE 1 2 4
MOLECULAR WEIGHT (G/GMOLE)     314.82
AQEOUS SOLUBILITY (PPM)     9.955
VAPOUR PRESSURE   (MM HG) .008646
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.98
                 MASS PART.      EQUI.PART.      AMOUNT            CONCENTRATION
                                                  (MOL)                (PPM)

AIR              .360382         1.22541E-6      36.0382           1.58901E-3

SOIL             .315753         .143155         31.5753           .147267

WATER            2.85733E-2      8.32787E-5      2.85733           1.28507E-4

BIOTA            9.74902E-5      .284141         9.74902E-3        .438455

SUSP SOLIDS      4.91172E-4      .28631          4.91172E-2        .294535

SEDIMENT         .294703         .28631          29.4703           .294535
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NAME OF CHEMICAL     TRIBROMOBENZENE   1 3 5
MOLECULAR WEIGHT (G/GMOLE)     314.82
AQEOUS SOLUBILITY (PPM)     .79
VAPOUR PRESSURE   (MM HG) .001788
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.98
                 MASS PART.      EQUI.PART.      AMOUNT            CONCENTRATION
                                                  (MOL)                (PPM)

AIR              .594359         3.19336E-6      59.4859           2.62288E-3

SOIL             .200001         .143155         20.0001           9.32806E-2

WATER            1.80986E-2      8.32785E-5      1.80986           8.13973E-5

BIOTA            6.17513E-5      .28414          6.17513E-3        .277722

SUSP SOLIDS      3.11113E-4      .286309         3.11113E-2        .186561

SEDIMENT         .186668         .286309         18.6668           .186561
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NAME OF CHEMICAL    TETRACHLOROBENZENE 1 2 3 4
MOLECULAR WEIGHT (G/GMOLE)     215.9
AQEOUS SOLUBILITY (PPM)     4.307
VAPOUR PRESSURE   (MM HG) .05994
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 5.05
                   MASS PART.     EQUI.PART.      AMOUNT         CONCENTRATION
                                                   (MOL)              (PPM)

AIR                 .8414          1.15398E-5      84.14          2.54423E-3

SOIL                7.88187E-2     .144134         7.88187        2.52103E-2

WATER               6.07075E-3     7.13662E-5      .607075        1.87239E-5

BIOTA               2.37543E-5     .27925          2.37543E-3     7.32651E-2

SUSP SOLIDS         1.22607E-4     .288267         1.22607E-2     5.04206E-2

SEDIMENT            7.35641E-2     .288267         7.35641        5.04206E-2
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NAME OF CHEMICAL    TETRACHLOROBENZENE 1 2 3 5
MOLECULAR WEIGHT (G/GMOLE)     215.9
AQEOUS SOLUBILITY (PPM)     3.5
VAPOUR PRESSURE   (MM HG) .12157
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 5.05
                   MASS PART.     EQUI.PART.      AMOUNT         CONCENTRATION
                                                   (MOL)              (PPM)

AIR                 .929779        2.88011E-5      92.9779        2.81148E-3

SOIL                3.48972E-2     .144131         3.48972        1.11619E-2

WATER               2.68784E-3     7.13649E-5      .268784        8.29006E-6

BIOTA               1.05173E-5     .279245         1.05173E-3     3.24383E-2

SUSP SOLIDS         5.42845E-5     .288262         5.42845E-3     2.23239E-2

SEDIMENT            3.25707E-2     .288262         3.25707        2.23239E-2
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NAME OF CHEMICAL    TETRACHLORO BENZENE 1 2 4 5   C6H2.CL4
MOLECULAR WEIGHT (G/MOLE)     215.91
AQUEOUS SOLUBILITY (PPM)      6
VAPOUR PRESSURE   (MM HG) .093
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 4.672
                         MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                          (MOL)              (PPM)

AIR                       .930543        2.95371E-5       93.0543         2.81392E-3

SOIL                      3.27758E-2     .138715          3.27758         1.04839E-2

WATER                     6.02791E-3     1.64003E-4       .602791         1.85926E-5

BIOTA                     1.12555E-5     .306232          1.12555E-3      3.47169E-2

SUSP SOLIDS               5.09846E-5     .27743           5.09846E-3      2.09678E-2

SEDIMENT                  3.05908E-2     .27743           3.05908         2.09678E-2
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NAME OF CHEMICAL     PENTACHLOROBENZENE    C6HCL5
MOLECULAR WEIGHT (G/GMOLE)      250.359
AQUEOUS SOLUBILITY (PPM)      .135
VAPOUR PRESSURE   (MM HG) .00582
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 5.188
                        MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                         (MOL)               (PPM)

AIR                      .933402        3.05661E-5      93.3402          3.27291E-3

SOIL                     3.34455E-2     .146032         3.34455          .012405

WATER                    1.87478E-3     5.26229E-5      .187478          6.70526E-6

BIOTA                    9.61061E-6     .269758         9.61061E-4       3.43729E-2

SUSP SOLIDS              5.20263E-5     .292063         5.20263E-3       .02481

SEDIMENT                 3.12158E-2     .292063         3.12158          .02481
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NAME OF CHEMICAL  HEXACHLOROBENZENE   C6CL6
MOLECULAR WEIGHT (G/GMOLE)    284.8I
AQUEOUS SOLUBILITY (PPM)   5E-3
VAPOUR PRESSURE ( MM HG)  2.IE-5
LOG OF OCTANOL-WATER PARTITION COEFFICIENT   5.23
                  MASS PART       EQUI. PART.      AMOUNT      CONCENTRATION
                                                    (MOL)           (PPM)

AIR               .585828         3.0888E-6        58.276       2.3368E-3
SOIL              .208540         .I46606-         20.854       0.08799
WATER             .0I06I2         4.796E-5         I.06I2       4.3I78E-5
BIOTA             5.906IE-5       .266919          5.906IE-3    .240302
SUSP.SOLIDS       3.2439E-4       .2932I2          3.2439E-2    .I7598
SEDIMENT          .I94637         .2932I2          I9.4637      .I7598
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NAME OF CHEMICAL    METHYL BENZENE   TOLUENE    C6H5.CH3
MOLECULAR WEIGHT (G/MOLE)      92.141
AQUOUS SOLUBILITY (PPM)      470
VAPOUR PRESSURE   (MM HG) 28.358
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.69
                  MASS PART.       EQUI.PART.      AMOUNT           CONCENTRATION
                                                   (MOL)              (PPM)

AIR                .995691         3.56296E-3      99.5691          1.28493E-3

SOIL               2.20047E-4      .104983         2.20047E-2       3.00376E-5

WATER              3.88265E-3      1.19088E-2      .388265          5.11073E-6

BIOTA              1.49840E-7      .459587         1.49840E-5       1.97235E-4

SUSP SOLIDS        3.42295E-7      .209976         3.42295E-5       6.00751E-5

SEDIMENT           2.05377E-4      .209976         2.05377E-2       6.00751E-5
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NAME OF CHEMICAL   O XYLENE   O METHYLTOLUENE   CH3.C6H4.CH3
MOLECULAR WEIGHT (G/GMOLE)    I06.I7
AQUEOUS SOLUBILITY   (PPM)    I75
VAPOUR PRESSURE (MM HG)   6.536
LOG OF OCTANOL-WATER PARTITION COEFFICIENT   3.I2
                   MASS PART       EQUI.PART.       AMOUNT        CONCENTRATION
                                                     (MOL)            (PPM)

AIR                0.99I325        8.08I4E-4        99.I325       I.474IE-3

SOIL               I.0428E-3       0.II33457        0.I0428       I.6402E-4

WATER              6.8360E-3       4.7768E-3        0.6836I       I.0368E-5

BIOTA              6.I207E-7       0.42768          6.I207E-5     9.2834E-4

SUSP SOLIDS        I.622IE-6       0.22669          I.622IE-4     3.2803E-4

SEDIMENT           9.7327E-4       0.22669          0.09733-      3.2803E-4
```

```
NAME OF CHEMICAL   M XYLENE   M METHYLTOLUENE   CH3.C6H4.CH3
MOLECULAR WEIGHT (G/GMOLE)   I06.I7
AQUEOUS SOLUBILITY (PPM)   I60.3I7
VAPOUR PRESSURE(MM HG)   8.284
LOG OF OCTANOL -WATER PARTITION COEFFICIENT   3.2
                    MASS PART.      EQUI.PART.      AMOUNT         CONCENTRATION
                                                     (MOL)            (PPM)

AIR                 .99467          I.I879E-3       99.4677         I.479IE-3
SOIL                7.2048E-4       .II473          .072049         I.I333E-4
WATER               3.9287E-3       4.02I8E-3       .392865         5.9586E-6
BIOTA               4.II37E-7       .42II29         4.II37E-5       6.2394E-4
SUSP SOLIDS         I.I208E-6       .229465         I.I208E-4       2.2665E-4
SEDIMENT            6.7245E-4       .229465         .067245         2.2665E-4
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NAME OF CHEMICAL   P XYLENE   P METHYLTOLUENE   CH3.C6H4.CH3
MOLECULAR WEIGHT (G/GMOLE)   I06.I7
AQUEOUS SOLUBILITY(PPM)   2I4.463
VAPOUR PRESSURE (MM HG)   8.74
LOG OF OCTANOL-WATER PARTITION COEFFICIENT   3.I8
                    MASS PART       EQUI. PART      AMOUNT         CONCENTRATION
                                                     (MOL)            (PPM)

AIR                 .993339         9.7822E-4       99.3339         I.4770E-3
SOIL                8.7I26E-4       .II4407         .087I26         I.3704E-4
WATER               4.9746E-3       4.I99IE-3       .49746          7.5450E-6
BIOTA               5.009IE-7       .42820          5.0050E-5       7.5972E-4
SUSP SOLIDS         I.3550E-6       .22880I         I.3553E-4       2.7408E-4
SEDIMENT            8.I3I8E-4       .22880I         .08I3I8         2.7408E-4
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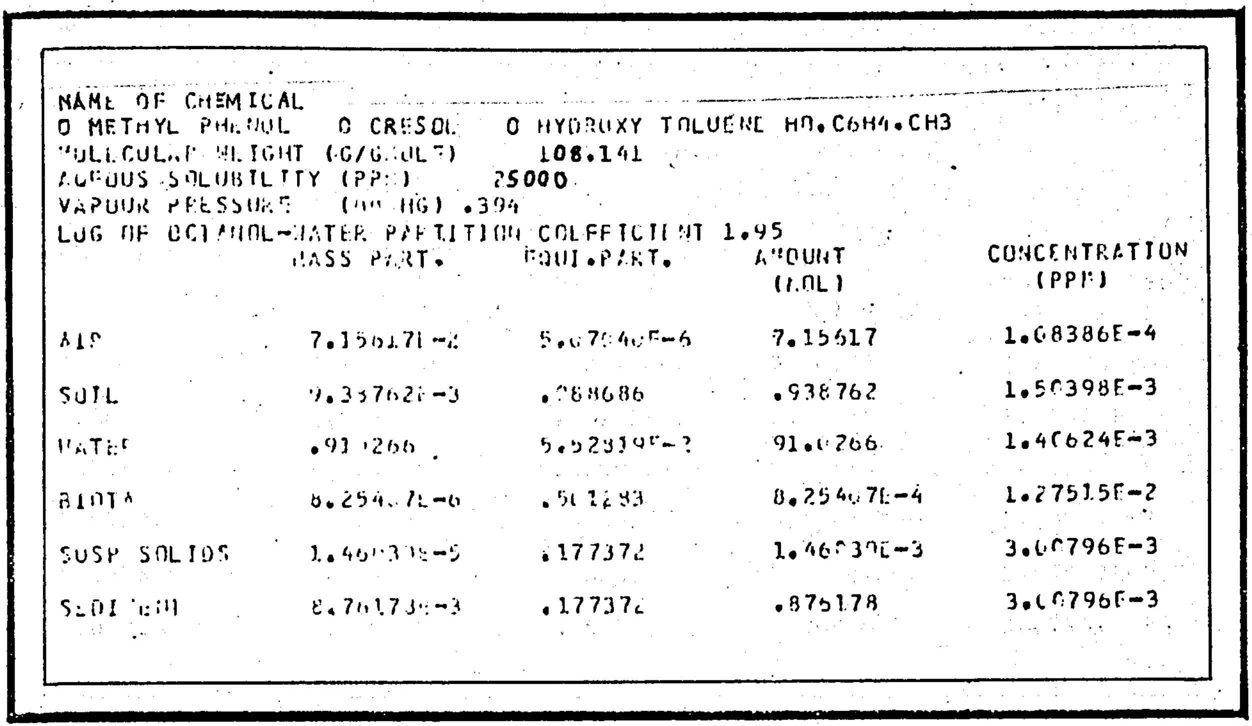

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NAME OF CHEMICAL
O METHYL PHENOL   O CRESOL   O HYDROXY TOLUENE HO.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)       108.141
AQUEOUS SOLUBILITY (PPM)      25000
VAPOUR PRESSURE   (MM HG) .394
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.95
                  MASS PART.     EQUI.PART.      AMOUNT          CONCENTRATION
                                                 (MOL)              (PPM)

AIR               7.15617E-2     5.67940E-6      7.15617          1.08386E-4

SOIL              9.38762E-3     .268686         .938762          1.50398E-3

WATER             .910266        5.52819E-2      91.0266          1.40624E-3

BIOTA             8.25407E-6     .501283         8.25407E-4       1.27515E-2

SUSP SOLIDS       1.46039E-5     .177372         1.46039E-3       3.00796E-3

SEDIMENT          8.75178E-3     .177372         .875178          3.00796E-3
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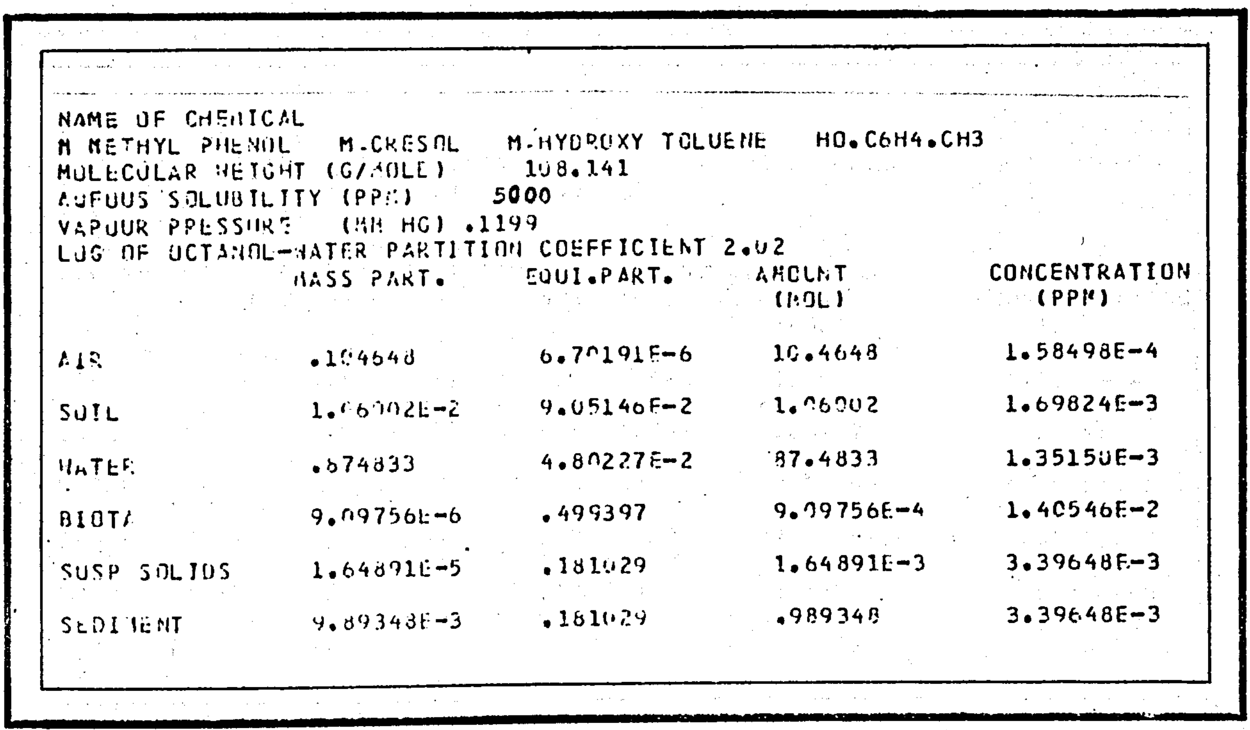

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NAME OF CHEMICAL
M METHYL PHENOL   M.CRESOL   M.HYDROXY TOLUENE   HO.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)      108.141
AQUEOUS SOLUBILITY (PPM)      5000
VAPOUR PRESSURE   (MM HG) .1199
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.02
                  MASS PART.     EQUI.PART.      AMOUNT          CONCENTRATION
                                                 (MOL)              (PPM)

AIR               .104648        6.70191E-6      10.4648          1.58498E-4

SOIL              1.06002E-2     9.05146E-2      1.06002          1.69824E-3

WATER             .874833        4.80227E-2      87.4833          1.35150E-3

BIOTA             9.09756E-6     .499397         9.09756E-4       1.40546E-2

SUSP SOLIDS       1.64891E-5     .181029         1.64891E-3       3.39648E-3

SEDIMENT          9.89348E-3     .181029         .989348          3.39648E-3
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NAME OF CHEMICAL
P METHYL PHENOL   P CRESOL   P HYDROXY TOLUENE   HO.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)      108.141
AQEOUS SOLUBILITY (PPM)     18000
VAPOUR PRESSURE   (MM HG) .1055
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.94
                      MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                       (MOL)              (PPM)

AIR                   2.78782E-2      1.92378E-6      2.78782          4.22238E-5

SOIL                  9.60985E-3      8.84191E-2      .960985          1.53958E-3

WATER                 .953519         5.63993E-2      95.3519          1.47306E-3

BIOTA                 8.47870E-6      .501505         8.47870E-4       1.30985E-2

SUSP SOLIDS           1.49487E-5      .176836         1.49487E-3       3.07917E-3

SEDIMENT              8.96919E-3      .176838         .696919          3.07917E-3
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NAME OF CHEMICAL
O METHYL ANILINE   O TOLUIDINE   O AMINO TOLUENE   NH2.C6H4.CH3
MOLECULAR WEIGHT (G/GMOLE)      107.157
AQEOUS SOLUBILITY (PPM)      15000
VAPOUR PRESSURE   (MM HG) .249
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.29
                      MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                       (MOL)              (PPM)

AIR                   7.55259E-2      1.52455E-5      7.55259          1.13349E-4

SOIL                  2.07677E-3      6.68941E-2      .207677          3.29690E-4

WATER                 .920453         .190597         92.0453          1.40904E-3

BIOTA                 2.29352E-6      .474914         2.29352E-4       3.51095E-3

SUSP SOLIDS           3.23053E-6      .133788         3.23053E-4       6.59380E-4

SEDIMENT              1.93832E-3      .133788         .193832          6.59380E-4
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NAME OF CHEMICAL
M METHYL ANILINE    M TOLUIDINE    M AMINO TOLUENE    NH2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)       107.157
AQEOUS SOLUBILITY (PPM)       25302
VAPOUR PRESSURE   (MM HG) .336
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.4
                   MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                    (MOL)               (PPM)

AIR                6.12735E-2      1.20579E-5      6.12735          9.19592E-5

SOIL               2.71325E-3      7.11911E-2      .271325          4.30731E-4

WATER              .933474         .157454         93.3474          1.42897E-3

BIOTA              2.88471E-6      .486579         2.88471E-4       4.41595E-3

SUSP SOLIDS        4.22060E-6      .142382         4.22060E-4       8.61461E-4

SEDIMENT           2.53236E-3      .142382         .253236          8.61461E-4
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NAME OF CHEMICAL
P METHYL ANILINE    P TOLUIDINE    P AMINO TOLUENE    NH2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)       107.157
AQEOUS SOLUBILITY (PPM)       7400
VAPOUR PRESSURE   (MM HG) .3025
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.39
                   MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                    (MOL)               (PPM)

AIR                .167329         3.77790E-5      16.7329          2.51127E-4

SOIL               2.35222E-3      7.08103E-2      .235222          3.73418E-4

WATER              .828117         .16026          82.8117          1.26769E-3

BIOTA              2.50953E-6      .485651         2.50953E-4       3.84162E-3

SUSP SOLIDS        3.65902E-6      .141621         3.65902E-4       7.46836E-4

SEDIMENT           2.19541E-3      .141621         .219541          7.46836E-4
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NAME OF CHEMICAL     O METHYL NITROBENZENE    NO2.C6H4.CH3
MOLECULAR WEIGHT (G/GMOLE)       137.141
AQUEOUS SOLUBILITY (PPM)       651
VAPOUR PRESSURE    (MM HG) .195
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.3
                    MASS PART.       EQUI.PART.       AMOUNT             CONCENTRATION
                                                      (MOL)                 (PPM)

AIR                 .644966          5.95248E-5       64.4966            1.23661E-3

SOIL                7.84638E-3       9.72627E-2       .784638            1.59416E-3

WATER               .339346          2.72549E-2       33.9346            6.65812E-4

BIOTA               6.11339E-6       .486862          6.11339E-4         1.19771E-2

SUSP SOLIDS         1.22055E-5       .194465          1.22055E-3         3.18833E-3

SEDIMENT            7.32329E-3       .194465          .732329            3.18833E-3
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```
NAME OF CHEMICAL     M METHYL NITRO BENZENE    M NITRO TOLUENE    NO2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)       137.141
AQUEOUS SOLUBILITY (PPM)       498
VAPOUR PRESSURE    (MM HG) .2093
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.42
                    MASS PART.       EQUI.PART.       AMOUNT             CONCENTRATION
                                                      (MOL)                 (PPM)

AIR                 .715165          6.54032E-5       71.5165            1.37365E-3

SOIL                8.18692E-3       9.98278E-2       .818692            1.66335E-3

WATER               .268988          2.10653E-2       26.8988            5.26990E-4

BIOTA               6.11974E-6       .47971           6.11974E-4         1.19895E-2

SUSP SOLIDS         1.27352E-5       .199656          1.27352E-3         3.32670E-3

SEDIMENT            7.64112E-3       .199656          .764112            3.32670E-3
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NAME OF CHEMICAL     P METHYL NITRO BENZENE   P NITRO TOLUENE   NO2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)      137.141
AQEOUS SOLUBILITY (PPM)      442
VAPOUR PRESSURE   (MM HG) .16996
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.37
                   MASS PART.      EQUI.PART.      AMOUNT             CONCENTRATION
                                                    (MOL)                 (PPM)

AIR                 .698017         6.64222E-5      69.8017            1.34071E-3

SOIL                7.78295E-3      9.87484E-2      .778295            1.58128E-3

WATER               .286918         2.34022E-2      28.6918            5.62117E-4

BIOTA               5.91913E-6      .482789         5.91913E-4         1.15965E-2

SUSP SOLIDS         1.21068E-5      .197497         1.21068E-3         3.16255E-3

SEDIMENT            7.26409E-3      .197497         .726409            3.16255E-3
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PHENOL FAMILY

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NAME OF CHEMICAL
PHENOL   HYDROXY BENZENE   CARBOLIC ACID   BENZENOL   C6H5.OH
MOLECULAR WEIGHT (G/MOLE)     94.114
AQEOUS SOLUBILITY (PPM)     86600
VAPOUR PRESSURE   (MM HG) .2948
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.46
                    MASS PART.      EQUI.PART.      AMOUNT         CONCENTRATION
                                                     (MOL)             (PPM)

AIR                 1.44711E-2      2.43834E-6      1.44711          1.90747E-5

SOIL                3.26783E-3      7.34161E-2      .326783          4.55628E-4

WATER               .979203         .141423         97.9203          1.31652E-3

BIOTA               3.40308E-6      .491495         3.40308E-4       4.57540E-3

SUSP SOLIDS         5.08329E-6      .146832         5.08329E-4       9.11255E-4

SEDIMENT            3.04998E-3      .146832         .304998          9.11255E-4
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NAME OF CHEMICAL     O CHLORO PHENOL    HO.C6H5.CL
MOLECULAR WEIGHT (G/MOLE)     128.563
AQEOUS SOLUBILITY (PPM)     29000
VAPOUR PRESSURE   (MM HG) 2.295
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.15
                    MASS PART.      EQUI.PART.      AMOUNT         CONCENTRATION
                                                     (MOL)             (PPM)

AIR                 .312679         2.01852E-5      31.2679          5.63010E-4

SOIL                1.08898E-2      9.37332E-2      1.08898          2.07411E-3

WATER               .666242         3.68656E-2      66.6242          1.22363E-3

BIOTA               8.93577E-6      .494448         8.93577E-4       1.64116E-2

SUSP SOLIDS         1.69396E-5      .187466         1.69396E-3       4.14821E-3

SEDIMENT            1.01638E-2      .187466         1.01638          4.14821E-3
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NAME OF CHEMICAL     M CHLORO PHENOL    HO.C6H5.CL
MOLECULAR WEIGHT (G/MOLE)      128.563
AQEOUS SOLUBILITY (PPM)     26000
VAPOUR PRESSURE   (MM HG) .276
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.5
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                 5.55249E-2      1.30994E-6      5.55249          9.99783E-5

SOIL                3.22744E-2      .101522         3.22744          6.14709E-3

WATER               .882004         1.78355E-2      88.2004          1.61990E-3

BIOTA               2.34677E-5      .474555         2.34677E-3       4.31011E-2

SUSP SOLIDS         5.02046E-5      .203043         5.02046E-3       1.22942E-2

SEDIMENT            3.01227E-2      .203043         3.01227          1.22942E-2
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NAME OF CHEMICAL     P CHLORO PHENOL    HO.C6H5.CL
MOLECULAR WEIGHT (G/MOLE)      128.563
AQEOUS SOLUBILITY (PPM)     27100
VAPOUR PRESSURE   (MM HG) .19
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.39
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                 .037917         1.08894E-6      3.7917           6.82734E-5

SOIL                2.59033E-2      .099189         2.59033          4.93364E-3

WATER               .911943         2.24487E-2      91.1943          1.67489E-3

BIOTA               1.95645E-5      .481605         1.95645E-3       3.59324E-2

SUSP SOLIDS         4.02940E-5      .198378         4.02940E-3       9.86727E-3

SEDIMENT            2.41764E-2      .198378         2.41764          9.86727E-3
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NAME OF CHEMICAL
O METHYL PHENOL   O CRESOL   O HYDROXY TOLUENE HO.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)      108.141
AQEOUS SOLUBILITY (PPM)      25000
VAPOUR PRESSURE   (MM HG) .394
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.95
                    MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR                 7.15617E-2     5.07040E-6     7.15617         1.08386E-4

SOIL                9.38762E-3     .088686        .938762         1.50398E-3

WATER               .910266        5.52819E-2     91.0266         1.40624E-3

BIOTA               8.25407E-6     .561283        8.25407E-4      1.27515E-2

SUSP SOLIDS         1.46030E-5     .177372        1.46030E-3      3.00796E-3

SEDIMENT            8.76178E-3     .177372        .876178         3.00796E-3
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NAME OF CHEMICAL
M METHYL PHENOL   M CRESOL   M HYDROXY TOLUENE   HO.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)     108.141
AQEOUS SOLUBILITY (PPM)     5000
VAPOUR PRESSURE   (MM HG) .1199
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.02
                    MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR                 .104648        6.70191E-6     10.4648         1.58498E-4

SOIL                1.06002E-2     9.05146E-2     1.06002         1.69824E-3

WATER               .874833        4.80227E-2     87.4833         1.35150E-3

BIOTA               9.09756E-6     .499397        9.09756E-4      1.40546E-2

SUSP SOLIDS         1.64891E-5     .181029        1.64891E-3      3.39648E-3

SEDIMENT            9.89348E-3     .181029        .989348         3.39648E-3
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NAME OF CHEMICAL
P METHYL PHENOL   P CRESOL   P HYDROXY TOLUENE   HO.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)     108.141
AQUEOUS SOLUBILITY (PPM)     18000
VAPOUR PRESSURE   (MM HG) .1055
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.94
                     MASS PART.     EQUI.PART.     AMOUNT         CONCENTRATION
                                                   (MOL)             (PPM)

AIR                  2.78782E-2     1.92378E-6     2.78782         4.22238E-5

SOIL                 9.60985E-3     8.84191E-2     .960985         1.53958E-3

WATER                .953519        5.63993E-2     95.3519         1.47306E-3

BIOTA                8.47870E-6     .501503        8.47870E-4      1.30985E-2

SUSP SOLIDS          1.49487E-5     .176838        1.49487E-3      3.07917E-3

SEDIMENT             8.96919E-3     .176838        .896919         3.07917E-3
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NAME OF CHEMICAL
M ETHYL PHENOL   1 ETHYL 3 HYDROXY  BENZENE   HO.C6H5.C2H5
MOLECULAR WEIGHT (G/MOLE)     122.168
AQUEOUS SOLUBILITY (PPM)     923.014
VAPOUR PRESSURE   (MM HG) .079
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.4
                     MASS PART.     EQUI.PART.     AMOUNT         CONCENTRATION
                                                   (MOL)             (PPM)

AIR                  .312325        1.23048E-5     31.2325         5.34400E-4

SOIL                 1.89234E-2     9.94038E-2     1.89234         3.42493E-3

WATER                .651046        2.19852E-2     65.1046         1.13624E-3

BIOTA                1.42433E-5     .480984        1.42433E-3      2.48583E-2

SUSP SOLIDS          2.94364E-5     .198808        2.94364E-3      6.84987E-3

SEDIMENT             1.76618E-2     .198808        1.76618         6.84987E-3
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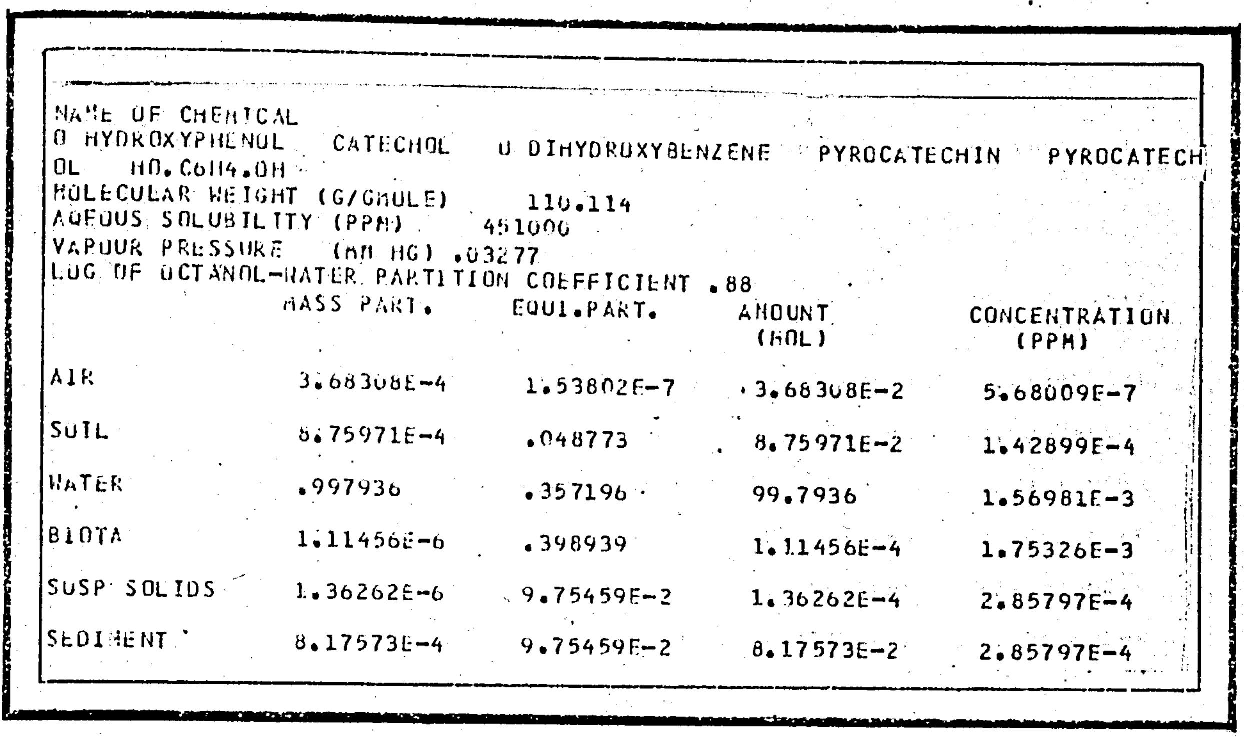

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NAME OF CHEMICAL
O HYDROXYPHENOL   CATECHOL   O DIHYDROXYBENZENE   PYROCATECHIN   PYROCATECH
OL   HO.C6H4.OH
MOLECULAR WEIGHT (G/GMOLE)      110.114
AQEOUS SOLUBILITY (PPM)      451000
VAPOUR PRESSURE    (MM HG) .03277
LOG OF OCTANOL-WATER PARTITION COEFFICIENT .88
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                    (MOL)               (PPM)

AIR                 3.68308E-4      1.53802E-7      3.68308E-2      5.68009E-7

SOIL                8.75971E-4      .048773         8.75971E-2      1.42899E-4

WATER               .997936         .357196         99.7936         1.56981E-3

BIOTA               1.11456E-6      .398939         1.11456E-4      1.75326E-3

SUSP SOLIDS         1.36262E-6      9.75459E-2      1.36262E-4      2.85797E-4

SEDIMENT            8.17573E-4      9.75459E-2      8.17573E-2      2.85797E-4
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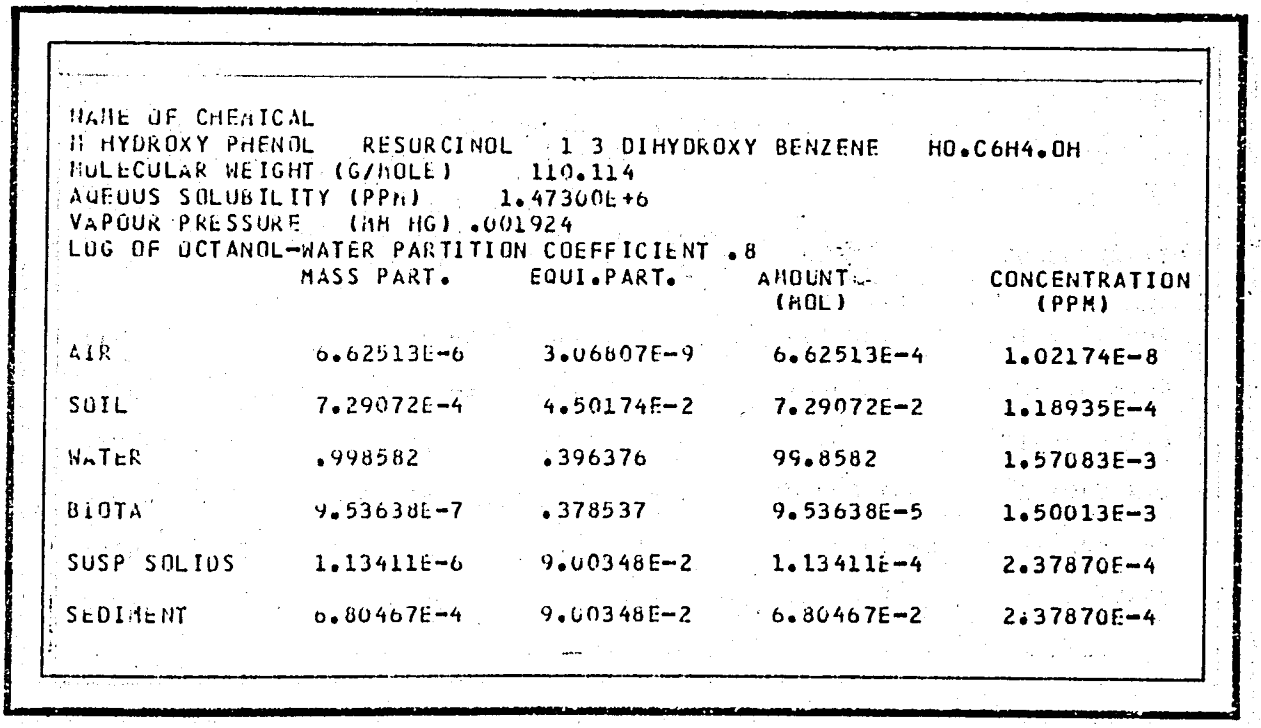

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NAME OF CHEMICAL
M HYDROXY PHENOL   RESORCINOL   1 3 DIHYDROXY BENZENE   HO.C6H4.OH
MOLECULAR WEIGHT (G/MOLE)      110.114
AQEOUS SOLUBILITY (PPM)      1.47300E+6
VAPOUR PRESSURE    (MM HG) .001924
LOG OF OCTANOL-WATER PARTITION COEFFICIENT .8
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                    (MOL)               (PPM)

AIR                 6.62513E-6      3.06807E-9      6.62513E-4      1.02174E-8

SOIL                7.29072E-4      4.50174E-2      7.29072E-2      1.18935E-4

WATER               .998582         .396376         99.8582         1.57083E-3

BIOTA               9.53638E-7      .378537         9.53638E-5      1.50013E-3

SUSP SOLIDS         1.13411E-6      9.00348E-2      1.13411E-4      2.37870E-4

SEDIMENT            6.80467E-4      9.00348E-2      6.80467E-2      2.37870E-4
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NAME OF CHEMICAL
P HYDROXY PHENOL   HYDROQUINONE   QUINOL   1 4 DIHYDROXY BENZENE   HO.C6H4.
OH
MOLECULAR WEIGHT (G/MOLE)      110.114
AQUEOUS SOLUBILITY (PPM)     80000
VAPOUR PRESSURE   (MM HG) 7.28700E-6
LOG OF OCTANOL-WATER PARTITION COEFFICIENT .59
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)             (PPM)

AIR                 4.62262E-7      2.72163E-10     4.62262E-5       7.12907E-10

SOIL                4.49789E-4      3.53092E-2      4.49789E-2       7.33748E-5

WATER               .999129         .504215         99.9129          1.57169E-3

BIOTA               6.32589E-7      .319239         6.32589E-5       9.95098E-4

SUSP SOLIDS         6.99671E-7      7.06185E-2      6.99671E-5       1.46750E-4

SEDIMENT            4.19803E-4      7.06185E-2      4.19803E-2       1.46750E-4
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NAME OF CHEMICAL      O NITRO PHENOL    HO.C6H4.NO2
MOLECULAR WEIGHT (G/MOLE)      139.114
AQUEOUS SOLUBILITY (PPM)     13500
VAPOUR PRESSURE   (MM HG) .188
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.79
                    MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)             (PPM)

AIR                 8.10058E-2      7.91073E-6      8.10058          1.57830E-4

SOIL                6.46759E-3      8.42135E-2      .646759          1.33294E-3

WATER               .906474         7.58768E-2      90.6474          1.80147E-3

BIOTA               6.00974E-6      .503048         6.00974E-4       1.19434E-2

SUSP SOLIDS         1.00607E-5      .168427         1.00607E-3       2.66587E-3

SEDIMENT            6.03642E-3      .168427         .603642          2.66587E-3
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ANILINE FAMILY

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NAME OF CHEMICAL     ANILINE    AMINO BENZENE    PHENYL AMINE    NH2.C6H5
MOLECULAR WEIGHT (G/MOLE)       93.13
AQUEOUS SOLUBILITY (PPM)      36600
VAPOUR PRESSURE    (MM HG) .4685
LOG OF OCTANOL-WATER PARTITION COEFFICIENT .9
                      MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                       (MOL)              (PPM)

AIR                   5.20359E-2      2.23039E-5      5.20359         6.78727E-5

SOIL                  8.69774E-4      4.97075E-2      8.69774E-2      1.20003E-4

WATER                 .94628          .347656         94.628          1.25896E-3

BIOTA                 1.09906E-6      .403784         1.09906E-4      1.46222E-3

SUSP SOLIDS           1.35298E-6      .099415         1.35298E-4      2.40006E-4

SEDIMENT              8.11790E-4      .099415         .081179         2.40006E-4
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NAME OF CHEMICAL      O CHLORO ANILINE    NH2.C6H4.CL
MOLECULAR WEIGHT (G/GMOLE)       127.579
AQUEOUS SOLUBILITY (PPM)      8760
VAPOUR PRESSURE    (MM HG) .254
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.9
                      MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                       (MOL)              (PPM)

AIR                   .143582         1.21599F-5      14.3582         2.56556E-4

SOIL                  7.73416E-3      8.73337E-2      .773416         1.46180E-3

WATER                 .841446         6.10815F-2      84.1446         1.53358E-3

BIOTA                 6.91873E-6      .502238         6.91873E-4      1.26098E-2

SUSP SOLIDS           1.20309E-5      .174667         1.20309E-3      2.92360E-3

SEDIMENT              7.21855E-3      .174667         .721855         2.92360E-3
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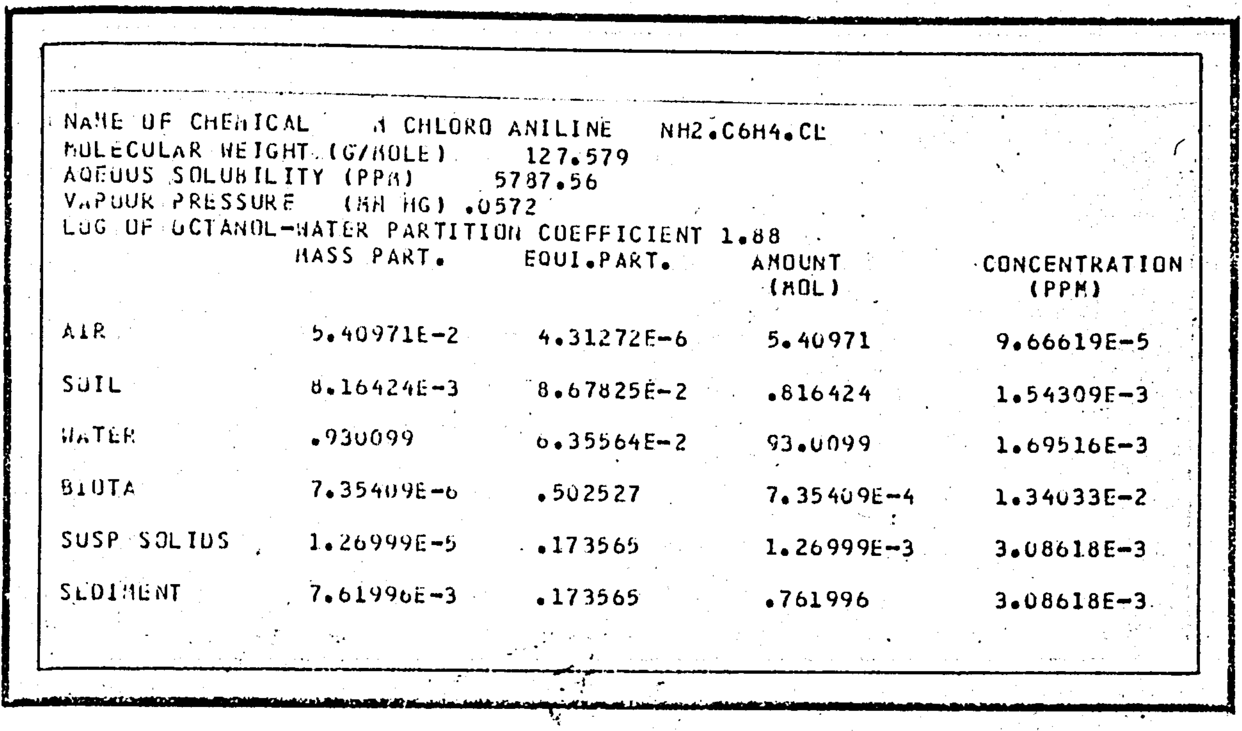

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NAME OF CHEMICAL     M CHLORO ANILINE    NH2.C6H4.CL
MOLECULAR WEIGHT (G/MOLE)      127.579
AQEUUS SOLUBILITY (PPM)      5787.56
VAPOUR PRESSURE    (MM HG) .0572
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.88
                   MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                    (MOL)              (PPM)

AIR                 5.40971E-2      4.31272E-6      5.40971          9.66619E-5

SOIL                8.16424E-3      8.67825E-2      .816424          1.54309E-3

WATER               .930099         6.35564E-2      93.0099          1.69516E-3

BIOTA               7.35409E-6      .502527         7.35409E-4       1.34033E-2

SUSP SOLIDS         1.26999E-5      .173565         1.26999E-3       3.08618E-3

SEDIMENT            7.61996E-3      .173565         .761996          3.08618E-3
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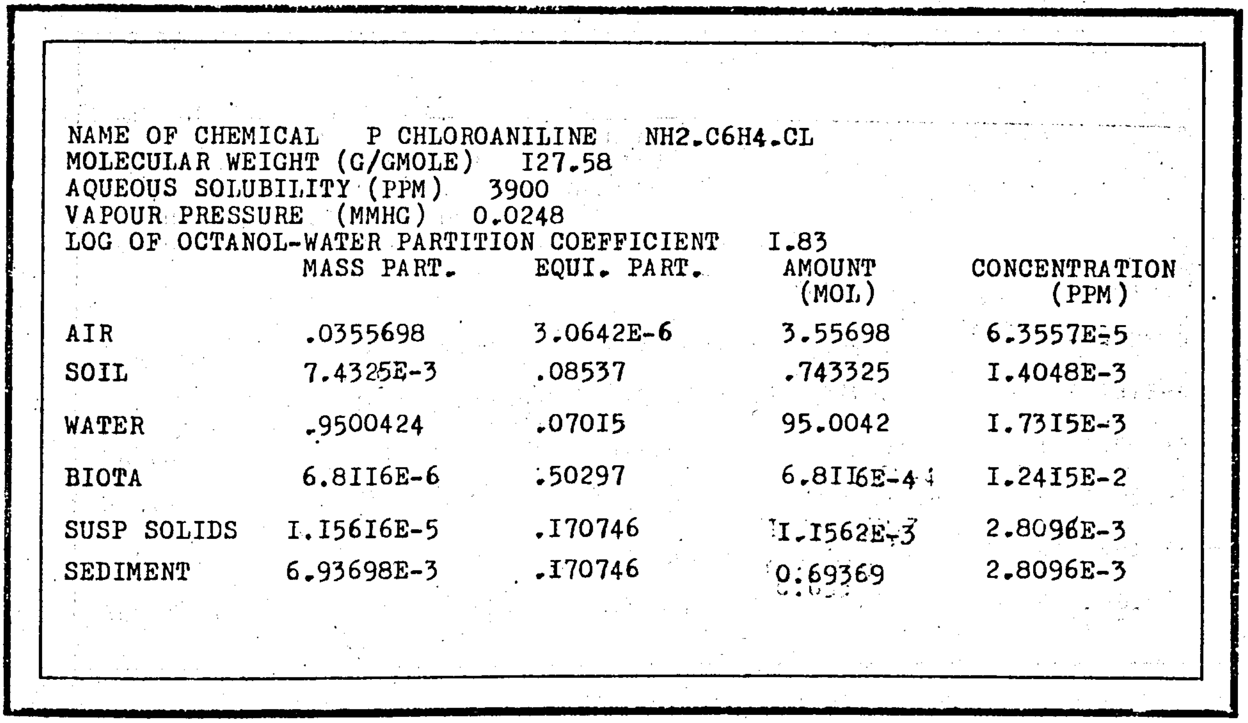

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NAME OF CHEMICAL    P CHLOROANILINE    NH2.C6H4.CL
MOLECULAR WEIGHT (G/GMOLE)   I27.58
AQUEOUS SOLUBILITY (PPM)   3900
VAPOUR PRESSURE  (MMHG)   0.0248
LOG OF OCTANOL-WATER PARTITION COEFFICIENT   I.83
                     MASS PART.      EQUI. PART.      AMOUNT      CONCENTRATION
                                                       (MOL)          (PPM)
AIR                  .0355698        3.0642E-6        3.55698      6.3557E-5
SOIL                 7.4325E-3       .08537           .743325      I.4048E-3

WATER                .9500424        .070I5           95.0042      I.73I5E-3

BIOTA                6.8II6E-6       .50297           6.8II6E-4    I.24I5E-2

SUSP SOLIDS         I.I56I6E-5       .I70746          I.I562E-3    2.8096E-3
SEDIMENT            6.93698E-3       .I70746          0.69369      2.8096E-3
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NAME OF CHEMICAL
O METHYL ANILINE    O TOLUIDINE    O AMINO TOLUENE    NH2.C6H4.CH3
MOLECULAR WEIGHT (G/GMOLE)      107.157
AQEOUS SOLUBILITY (PPM)      15000
VAPOUR PRESSURE   (MM HG) .249
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.29
                   MASS PART.       EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                7.55259E-2       1.82455E-5      7.55259          1.13349E-4

SOIL               2.07677E-3       6.68941E-2      .207677          3.29690E-4

WATER              .920453          .190597         92.0453          1.40904E-3

BIOTA              2.29352E-6       .474914         2.29352E-4       3.51095E-3

SUSP SOLIDS        3.23053E-6       .133788         3.23053E-4       6.59380E-4

SEDIMENT           1.93832E-3       .133788         .193832          6.59380E-4
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NAME OF CHEMICAL
M METHYL ANILINE    M TOLUIDINE    M AMINO TOLUENE    NH2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)      107.157
AQEOUS SOLUBILITY (PPM)      25302
VAPOUR PRESSURE    (MM HG) .336
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.4
                   MASS PART.       EQUI.PART.      AMOUNT          CONCENTRATION
                                                     (MOL)              (PPM)

AIR                6.12735E-2       1.20579E-5      6.12735          9.19592E-5

SOIL               2.71325E-3       7.11911E-2      .271325          4.30731E-4

WATER              .933474          .157454         93.3474          1.42897E-3

BIOTA              2.88471E-6       .486579         2.88471E-4       4.41595E-3

SUSP SOLIDS        4.22060E-6       .142382         4.22060E-4       8.61461E-4

SEDIMENT           2.53236E-3       .142382         .253236          8.61461E-4
```
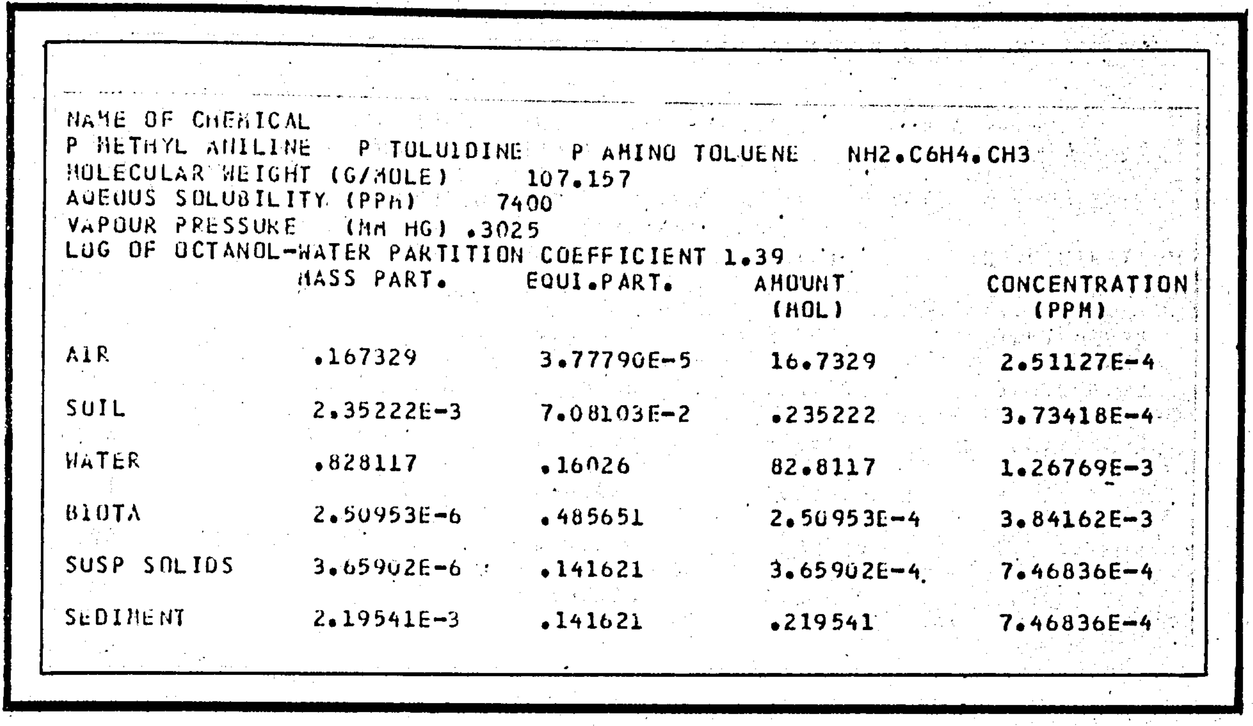
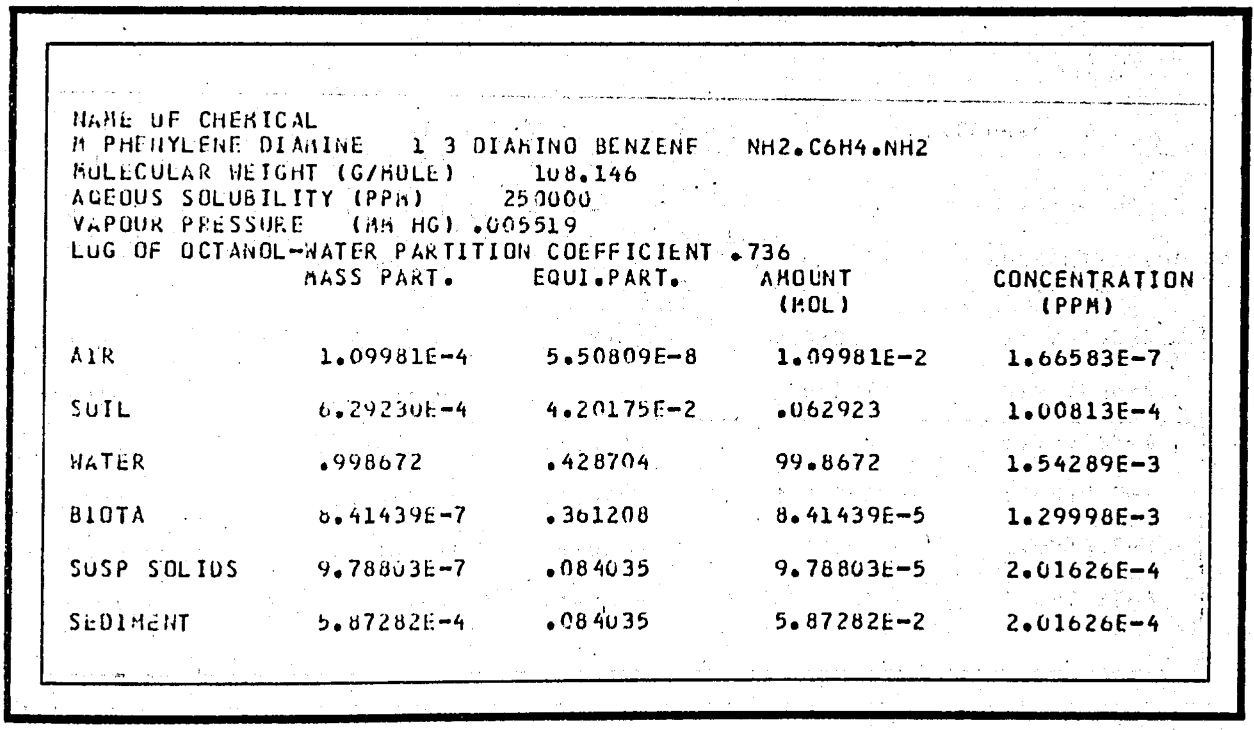



```
NAME OF CHEMICAL
P METHYL ANILINE   P TOLUIDINE   P AMINO TOLUENE   NH2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)     107.157
AQEOUS SOLUBILITY (PPM)     7400
VAPOUR PRESSURE   (MM HG) .3025
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.39
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)             (PPM)

AIR                .167329        3.77790E-5      16.7329         2.51127E-4

SOIL              2.35222E-3      7.08103E-2      .235222         3.73418E-4

WATER              .828117         .16026         82.8117         1.26769E-3

BIOTA             2.50953E-6       .485651        2.50953E-4      3.84162E-3

SUSP SOLIDS       3.65902E-6       .141621        3.65902E-4      7.46836E-4

SEDIMENT          2.19541E-3       .141621        .219541         7.46836E-4
```



```
NAME OF CHEMICAL
M PHENYLENE DIAMINE   1 3 DIAMINO BENZENE   NH2.C6H4.NH2
MOLECULAR WEIGHT (G/MOLE)     108.146
AQEOUS SOLUBILITY (PPM)     250000
VAPOUR PRESSURE   (MM HG) .005519
LOG OF OCTANOL-WATER PARTITION COEFFICIENT .736
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)             (PPM)

AIR               1.09981E-4      5.50809E-8      1.09981E-2      1.66583E-7

SOIL              6.29230E-4      4.20175E-2      .062923         1.00813E-4

WATER              .998672         .428704        99.8672         1.54289E-3

BIOTA             8.41439E-7       .361208        8.41439E-5      1.29998E-3

SUSP SOLIDS       9.78803E-7       .084035        9.78803E-5      2.01626E-4

SEDIMENT          5.87282E-4       .084035        5.87282E-2      2.01626E-4
```

```
NAME OF CHEMICAL     O NITRO ANILINE    O NITRANILINE    NH2.C6H4.NO2
MOLECULAR WEIGHT (G/MOLE)      138.13
AQUEOUS SOLUBILITY (PPM)      1212
VAPOUR PRESSURE    (MM HG) .004087
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.36
                    MASS PART.      EQUI.PART.      AMOUNT             CONCENTRATION
                                                     (MOL)                 (PPM)

AIR                 .020028         5.99001E-7      2.0028             3.87461E-5

SOIL                2.47098E-2      9.85366E-2      2.47098            5.05654E-3

WATER               .932142         .023896         93.2142            1.83938E-3

BIOTA               1.88574E-5      .48342          1.88574E-3         3.72111E-2

SUSP SOLIDS         3.84375E-5      .197073         3.84375E-3         1.01131E-2

SEDIMENT            2.30625E-2      .197073         2.30625            1.01131E-2
```

```
NAME OF CHEMICAL     M NITRO ANILINE    M NITRANILINE    NH2.C6H4.NO2
MOLECULAR WEIGHT (G/MOLE)      138.13
AQUEOUS SOLUBILITY (PPM)      1210
VAPOUR PRESSURE    (MM HG) 1.21490E-3
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.37
                    MASS PART.      EQUI.PART.      AMOUNT             CONCENTRATION
                                                     (MOL)                 (PPM)

AIR                 6.32381E-3      1.23902E-6      .632381            1.22340E-5

SOIL                2.68137E-3      .070048         .268137            5.48708E-4

WATER               .988485         .166006         98.8485            1.95056E-3

BIOTA               2.88052E-6      .483753         2.88052E-4         5.68408E-3

SUSP SOLIDS         4.17102E-6      .140096         4.17102E-4         1.09742E-3

SEDIMENT            2.50261E-3      .140096         .250261            1.09742E-3
```

```
NAME OF CHEMICAL     P NITRO ANILINE   P NITRANILINE   NH2.C6H4.NO2
MOLECULAR WEIGHT (G/MOLE)      138.13
AQUEOUS SOLUBILITY (PPM)      22200
VAPOUR PRESSURE   (MM HG) 2.98980E-4
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.39
                         MASS PART.     EQUI.PART.     AMOUNT          CONCENTRATION
                                                        (MOL)              (PPM)

AIR                      8.53344E-5     1.60446E-8     8.53344E-3      1.65087E-7

SOIL                     2.82467E-3     .070813        .282467         5.78033E-4

WATER                    .994446        .160266        99.4446         1.96233E-3

BIOTA                    3.01357E-6     .485669        3.01357E-4      5.94663E-3

SUSP SOLIDS              4.39394E-6     .141626        4.39394E-4      1.15607E-3

SEDIMENT                 2.63636E-3     .141626        .263636         1.15607E-3
```

NITROBENZENE FAMILY

```
NAME OF CHEMICAL    NITRO BENZENE   C6H5.NO2
MOLECULAR WEIGHT (G/MOLE)      123.114
AQUEOUS SOLUBILITY (PPM)     2050
VAPOUR PRESSURE   (MM HG) .265
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.85
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR                .419501         5.77592E-5      41.9501         7.23340E-4

SOIL               4.68118E-3      8.59374E-2      .468118         8.53805E-4

WATER              .571437         6.74388E-2      57.1437         1.00503E-3

BIOTA              4.26058E-6      .502817         4.26058E-4      7.49338E-3

SUSP SOLIDS        7.28183E-6      .171875         7.28183E-4      1.70761E-3

SEDIMENT           4.36910E-3      .171875         .43691          1.70761E-3
```

```
NAME OF CHEMICAL     O METHYL NITROBENZENE    NO2.C6H4.CH3
MOLECULAR WEIGHT (G/GMOLE)      137.141
AQUEOUS SOLUBILITY (PPM)     650
VAPOUR PRESSURE   (MM HG) .195
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.3
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR                .644966         5.99248E-5      64.4966         1.23881E-3

SOIL               7.84638E-3      9.72027E-2      .784638         1.59416E-3

WATER              .339846         2.70649E-2      33.9846         6.65812E-4

BIOTA              6.11339E-6      .486862         6.11339E-4      1.19771E-2

SUSP SOLIDS        1.22055E-5      .194405         1.22055E-3      3.18833E-3

SEDIMENT           7.32329E-3      .194405         .732329         3.18833E-3
```

```
NAME OF CHEMICAL    M METHYL NITRO BENZENE    M NITRO TOLUENE    NO2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)      137.141
AQEOUS SOLUBILITY (PPM)      498
VAPOUR PRESSURE    (MM HG) .2093
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.42
                     MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                      (MOL)               (PPM)

AIR                  .715165         6.54032E-5      71.5165           1.37365E-3

SOIL                 8.18692E-3      9.98278E-2      .818692           1.66335E-3

WATER                .268988         2.10853E-2      26.8988           5.26990E-4

BIOTA                6.11974E-6      .47971          6.11974E-4        1.19895E-2

SUSP SOLIDS          1.27352E-5      .199656         1.27352E-3        3.32670E-3

SEDIMENT             7.64112E-3      .199656         .764112           3.32670E-3
```

```
NAME OF CHEMICAL    P METHYL NITRO BENZENE    P NITRO TOLUENE    NO2.C6H4.CH3
MOLECULAR WEIGHT (G/MOLE)      137.141
AQEOUS SOLUBILITY (PPM)      442
VAPOUR PRESSURE    (MM HG) .16998
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.37
                     MASS PART.      EQUI.PART.      AMOUNT           CONCENTRATION
                                                      (MOL)               (PPM)

AIR                  .698017         6.64222E-5      69.8017           1.34071E-3

SOIL                 7.78295E-3      9.87484E-2      .778295           1.58128E-3

WATER                .286918         2.34022E-2      28.6918           5.62117E-4

BIOTA                5.91913E-6      .482789         5.91913E-4        1.15965E-2

SUSP SOLIDS          1.21068E-5      .197497         1.21068E-3        3.16255E-3

SEDIMENT             7.26409E-3      .197497         .726409           3.16255E-3
```

```
NAME OF CHEMICAL     O HYDROXY NITRO BENZENE    O NITRO PHENOL    NO2.C6H4.OH
MOLECULAR WEIGHT (G/MOLE)      139.114
AQEOUS SOLUBILITY (PPM)     2100
VAPOUR PRESSURE    (MM HG) .188
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.79
                 MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                  (MOL)              (PPM)

AIR               .361697         5.08525E-5      36.1697         7.04721E-4

SOIL              4.49217E-3      8.42099E-2      .449217         9.25814E-4

WATER             .629607         7.58736E-2      62.9607         1.25125E-3

BIOTA             4.17417E-6      .503026         4.17417E-4      8.29550E-3

SUSP SOLIDS       6.98783E-6      .16842          6.98783E-4      1.85163E-3

SEDIMENT          4.19270E-3      .16842          .41927          1.85163E-3
```

```
NAME OF CHEMICAL
O AMINO NITRO BENZENE   O NITRO ANILINE   O NITRANILINE   NO2.C6H4.NH2
MOLECULAR WEIGHT (G/MOLE)      138.13
AQEOUS SOLUBILITY (PPM)     1212
VAPOUR PRESSURE    (MM HG) .004087
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 2.36
                 MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                  (MOL)              (PPM)

AIR               .020028         5.99001E-7      2.0028          3.87461E-5

SOIL              2.47098E-2      9.85366E-2      2.47098         5.05654E-3

WATER             .932142         .023896         93.2142         1.83938E-3

BIOTA             1.88574E-5      .48342          1.88574E-3      3.72111E-2

SUSP SOLIDS       3.84375E-5      .197073         3.84375E-3      1.01131E-2

SEDIMENT          2.30625E-2      .197073         2.30625         1.01131E-2
```

```
NAME OF CHEMICAL
M AMINO NITRO BENZENE   M NITRO ANILINE   M NITRANILINE   NO2.C6H4.NH2
MOLECULAR WEIGHT (G/MOLE)      138.13
AQEOUS SOLUBILITY (PPM)      1210
VAPOUR PRESSURE    (MM HG) 1.21490E-3
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.37
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR               6.32381E-3      1.23902E-6      .632381          1.22340E-5

SOIL              2.68137E-3      .070048         .268137          5.48708E-4

WATER             .988485         .166006         98.8485          1.95056E-3

BIOTA             2.88052E-6      .483753         2.88052E-4       5.68408E-3

SUSP SOLIDS       4.17102E-6      .140096         4.17102E-4       1.09742E-3

SEDIMENT          2.50261E-3      .140096         .250261          1.09742E-3
```

```
NAME OF CHEMICAL
P AMINO NITRO BENZENE   P NITRO ANILINE   P NITRANILINE   NO2.C6H4.NH2
MOLECULAR WEIGHT (G/MOLE)      138.13
AQUEOUS SOLUBILITY (PPM)      22200
VAPOUR PRESSURE    (MM HG) 2.98980E-4
LOG OF OCTANOL-WATER PARTITION COEFFICIENT 1.39
                  MASS PART.      EQUI.PART.      AMOUNT          CONCENTRATION
                                                   (MOL)              (PPM)

AIR               8.53344E-5      1.60446E-8      8.53344E-3       1.65087E-7

SOIL              2.82467E-3      .070813         .282467          5.78033E-4

WATER             .994446         .160266         99.4446          1.96233E-3

BIOTA             3.01357E-6      .485669         3.01357E-4       5.94663E-3

SUSP SOLIDS       4.39394E-6      .141626         4.39394E-4       1.15607E-3

SEDIMENT          2.63636E-3      .141626         .263636          1.15607E-3
```

APPENDIX II

PHYSICAL AND CHEMICAL PROPERTIES OF BENZENE AND SUBSTITUTED BENZENES

TABLE A.2.1 Compilation of Physical and Chemical Properties for Benzene and 72 Substituted Benzenes

COMPOUND	MW Molecular weight g/mole	S Water Solubility g/m^3 (at 25^oC)	Ref	P Vapor Pressure mm Hg (at 25^oC)	Ref	Kow n-octanol water partition coefficient	Ref	Log Kow Log of n-octanol water partition coefficient	Ref
MONOSUBSTITUTED BENZENE FAMILY									
Benzene	78.114	1790	(7.22)	94.970	(22)	135	(6)	2.13	(17,19,26)
(Benzol)		1740	(22)	95.114	(calc2)				
C_6H_6		1780	(6,19)	95.044	(calc4)				
		1788.8	(20)	100.525	(calc5)				
		1789.6	(16,24)	95.044	(calc6)				
		1781.3	(26)						
		1789.5	(26)						
		1749.8	(23)						
Fluorobenzene	96.106	1553	(19)	76.523	(calc4)	186.21	(17)	2.27	(17)
$C_6H_5.F$		1540(30^o)	(14,17)	82.502	(calc5)				(calc7)
		1558.7	(16,24)	77.819	(calc6)				
Chlorobenzene	112.56	294.92	(20)	11.856	(28)	690	(6)	2.84	(17)
$C_6H_5.Cl$		480	(1)	11.8	(1)			2.84	(calc8)
		488	(12,13)	11.75	(13)				
		472	(19)	12.1	(calc2)				
		490(20^o)	(8)	11.967	(calc4)				
		488(30^o)	(17)	11.744	(calc5)				
		502.79	(16.24)	11.656	(calc6)				
		448	(6)						

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	Log Kow	Ref
Bromobenzene	157.02	410.6	(19)	3.9330	(calc2)	977.24	(calc7,17)	2.99	(calc7,17)
$C_6H_5.Br$		446	(6)	4.1389	(calc4)	900	(6)	2.95	(6)
		446(30°)	(12,17)	4.0772	(calc5)			3.07	(calc8)
		359.7	(16,24)	4.2286	(calc6)				
				4.1420	(28)				
Iodobenzene	204.01	340	(14,17,19)	0.9543	(calc2)	1778.3	(13,17)	3.25	(37,17)
$C_6H_5.I$		228.9	(16,24)	0.9903	(calc4)	2290.9	(16,calc8)	3.36	(16)(calc8)
				0.9221	(calc5)				
		200.76	(20)	1.0611	(calc6)				
				0.988	(28)				
Toluene	92.141	515	(7,13,19)	28.47	(22)	489.77	(calc7)	2,69	(17,19,26)
(Methyl benzene)		627	(22)	28.12	(28)	490	(7)		(calc7)
$C_6H_5.CH_3$		470	(17,25)	30	(25)				
		530	(22)	28.5	(13)				
		570	(12)	28.45	(calc2)				
		514.58	(26)	29.108	(calc5)				
		535.12	(26)	28.358	(calc6)				
		507.52	(26)						
		578.65	(20)						
Ethyl benzene	106.17	152	(13,19)	9.6	(13)	1412.5	(19,26,37)	3.15	(19,26,37)
$C_6H_5.C_2H_5$		100	(8)	9.494	(22)				
		152.1	(26)	9.88	(28)				
		208	(22)						
		186.86	(20						

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
n-Propyl benzene $C_6H_5.C_3H_7$	120.20	55	(19)	3.4276	(28)	4786.3	(19,26)	3.68	(19,26)
Isopropyl benzene $C_6H_5.C_3H_7$	120.20	50 49.99 65.3	(13,19) (26) (26)	4.6	(13)	4570.9	(19,26,37)	3.66	(19,26,37)
Butyl benzene $C_6H_5.C_4H_9$	134.22	5000	(13)	1.165 1.1	(cal6) (13)	12882	(37)	1.94	(calc9)
Benzyl alcohol (Phenyl carbinol) (Hydroxy Toluene) $C_6H_5.CH_2OH$	108.14	$4x10^4$ (17°)	(8,15)	0.0865 0.06	(calc2) (calc6)	12.59	(calc7)	1.1	(calc7)
Acetophenone (Acetyl benzene) (Methyl phenyl ketone) $C_6H_5.COCH_3$	120.15	$15.3x10^3$	(calc1)	0.3021	(calc3)	38.019	(calc7)	1.58	(calc7)

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
Phenol (Hydroxybenzene) (Carbolic acid) (Benzenol)	94.11	8.66x10^4 9.3 x10^4 8.2 x10^4 8.2 x10^4	(13) (15) (7) (8)	0.3513 0.2948 0.41	(calc2) (calc6) (13)	29 34.674	(7) (calc8)	1.46 1.54	(calc7) (calc8)
Anisole (methylphenylether) $C_6H_5.OCH_3$	108.14	1.04x10^4	(13)	3.372 4.2	(calc2) (13)	128.82	(calc7)	2.11	(calc7)
Aniline (Aminobenzene) $C_6H_5.NH_2$	93.13	3.66x10^4 3.38x10^4 3.7 x10^4 3.6 x10^4(18^9)	(6) (13) (15) (8)	0.6250 0.4685	(calc2) (calc6)	7.943 7	(calc7) (6)	0.9 1.0	(calc7) (calc8)
N,N-Dimethyl aniline $C_6H_5.N(CH_3)_2$	121.18	1.25x10^3	(calc1)	0.7418	(calc6)	204.17	(calc7)	2.31	(calc7)

TABLE A.2.1 - Continued...

COMPOUND	MW	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
Nitrobenzene	123.11	2050	(12)	0.265	(calc6)	70.79	(calc7)	1.85	(calc7)
$C_6H_5.NO_2$		1780	(6)	0.4134	(calc3)	62	(6)	1.79	(6)
		1900	(8)					1.82	calc8
		2092	(23)						
HALOBENZENE FAMILY									
Fluorobenzene	96.106	1553	(19)	76.523	(calc4)	186.21	(calc7)	2.27	(17)(calc7)
$C_6H_5.F$		1540(30^{o})	(14,17)	82.502	(calc5)				
		1558.7	(16,24)	77.819	(calc6)				
Chlorobenzene	112.56	294.92	(20)	11.856	(28)	690	(6)	2.84	(17)
$C_6H_5.Cl$		480	(1)	11.8	(1)				
		488	(12,13)	11.75	(13)				
		472	(19)	12.1	(calc2)				
		490(20^{o})	(8)	11.967	(calc4)				
		448(30^{o})	(17)						
		502.79	(16,24)	11.744	(calc5)				
		448	(6)	11.656	(calc6)				
Bromobenzene	157.02	410.6	(19)	3.9330	(calc2)	997.24	(17)	2.99	(17)
$C_6H_5.Br$		446	(6)	4.1389	(calc4)	900	(6)	2.95	(calc7)
		446(30^{o})	(12,17)	4.0772	(calc5)				
		359.7	(16,24)	4.2286	(calc6)				
				4.1420	(28)				

TABLE A.2.1 - Continued...

COMPOUND	MW	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
Iodobenzene	204.03	340 228.9 200.76	(14,17,19) (16,24) (20)	0.9543 0.9903 0.9281 1.0611 0.988	(calc2) (calc4) (calc5) (calc6) (28)	1778.28 2290.87	(17,37) (16)	3.25 3.36	(17)(37) (16)
o-Difluorobenzene $C_6H_4.F_2$	114.09	1140.9	(16,24)	62.596	(calc5)	389.04	(16)	2.59	(16)
m-Difluorobenzene $C_6H_4.F_2$	114.09	1140.9	(16,24)	89.686	(calc5)	380.19	(16)	2.58	(16)
p-Difluorobenzene $C_6H_4.F_2$	114.09	1224.4	(16,24)	70.614	(calc5)	380.19	(16)	2.58	(16)
o-Dichlorobenzene $C_6H_4.Cl_2$	147.01	150 260 92.757 155.83 92.324	(18) (13) (16,24) (23) (20)	1.4668 1.28 1.4793 1.3342 1.3928	(28) (13) (calc4) (calc5) (calc6)	3890.5	(16)	3.59 3.4	(16) (18)
m-Dichlorobenzene $C_6H_4.Cl_2$	147.01	120 119.49 133.49 124.52	(18) (16,24) (23) (20)	2.3028 1.9884 1.8857 2.2435	(28) (calc4) (calc5) (calc6)	3890.5	(16)	3.59 3.4	(16) (18)

TABLE A.2.1 - Continued...

COMPOUND	MW	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
p-Dichlorobenzene	147.01	79	(1,6,17,18,25)	0.6749	(28)	2450	(6)	3.389	(6,17)
$C_6H_4.Cl_2$				1.6924	(calc2)	2398.8	(35)	3.38	(35)
		77(30°)	(12)	1.8094	(calc4)				
		90.646	(16,24)	0.9508	(calc5)	2511.9	(18)	3.4	(18)
		73.8	(23)	1.9261	(calc6)				
		30.873	(20)						
o-Dibromobenzene $C_6H_4.Br_2$	235.92	74.6	(16,24)	0.1953 0.2422	(calc2) (calc5)	11749	(16)	4.07	(16)
m-Dibromobenzene $C_6H_4.Br_2$	235.92	98.347	(16,24)	0.4279(35°) 0.2261	(28) (calc5)	11749	(16)	4.07	(16)
p-Dibromobenzene $C_6H_4.Br_2$	235.92	20.08	(16,24)	0.1611 0.0524	(28) (calc5)	11749	(16)	4.07	(16)
o-Diiodobenzene $C_6H_4.I_2$	329.91	18.984	(16,24)	7.26×10^{-3}	(calc5)	44668	(16)	4.65	(16)
m-Diiodobenzene $C_6H_4.I_2$	329.91	8.8796	(16,24)	5.68×10^{-3}	(calc5)	43652	(16)	4.64	(16)
p-Diiodobenzene $C_6H_4.I_2$	329.91	1.855	(16,24)	6.97×10^{-4}	(calc5)	43652	(16)	4.64	(16)
o-Bromochlorobenzene $C_6H_4.BrCl$	191.46	123.62	(16,24)	0.4425	(calc5)	6760.8	(16)	3.83	(16)
m-Bromochlorobenzene $C_6H_4.BrCl$	191.46	118.5	(16,24)	0.6465	(calc5)	6760.8	(16)	3.83	(16)

TABLE A.2.1 - Continued...

COMPOUND	MW	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
p-Bromochlorobenzene $C_6H_4.BrCl$	191.46	44.882	(16,24)	0.2424 0.6331 0.2584	(calc5) (calc6) (28)	6760.8	(16)	3.83	(16)
p-Bromoiodobenzene $C_6H_4.BrI$	282.91	7.7919	(16)	$9.23x10^{-3}$	(calc5)	22909	16	4.36	(16)
o-Chloroiodobenzene $C_6H_4.ClI$	238.46	68.773	(16,24)	0.1012	(calc5)	13183	(16)	4.12	(16)
m-Chloroiodobenzene $C_6H_4.ClI$	238.46	67.207	(16)	0.1262	(calc5)	13183	(16)	4.12	(16)
p-Chloroiodobenzene $C_6H_4.ClI$	238.46	22.254	(16,24)	$7.04x10^{-2}$	(calc5)	13183	(16)	4.12	(16)
1,2,3-Trichlorobenzene $C_6H_3.Cl_3$	181.46	31.532 12.267	(16) (20)	0.3961 0.2098 0.1194	(calc6) (28) (calc5)	18621	(16)	4.27	(16)
1,2,4-Trichlorobenzene $C_6H_3.Cl_3$	181.46	30 34.574 46.091	(6,7) (24,16) (20)	0.4265 0.2809 0.2903 0.45	(calc6) (calc5) (calc2) (28)	$15x10^3$	(6)	4.18 4.27	(calc7) (16)
1,3,5-Trichlorobenzene $C_6H_3.Cl_3$	181.46	6.588 4.119	(16) (20)	0.5776 0.1537 0.8363	(28) (calc5) (calc6)	18621	(16)	4.27	(16)
1,2,4-Tribromobenzene $C_6H_3.Br_3$	314.82	9.955	(16)	$8.65x10^{-3}$	(calc5)	95499	(16)	4.98	(16)
1,3,5-Tribromobenzene $C_6H_3.Br_3$	314.82	0.79	(16)	$1.79x10^{-3}$	(calc5)	95499	(16)	4.98	(16)

TABLE A.2.1 - Continued...

COMPOUND	MW	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
1,2,3,4 tetrachlorobenzene $C_6H_2.Cl_4$	215.91	4.307 12.199	(16) (20)	0.0599 0.023 0.0391	(calc6) (calc5) (28)	11.22x10^4	(16)	5.05	(16)
1,2,3,5 tetrachlorobenzene $C_6H_2.Cl_4$	215.91	3.5 4.0159 4.219	(16) (23) (20)	0.1216 0.0734 0.0293	(calc6) (28) (calc5)	11.22x10^4	(16)	5.05	(16)
1,2,4,5, tetrachlorobenzene $C_6H_2.Cl_4$	215.91	6 0.5947 2.353	(6) (16,24) (20)	0.093 5.4x10^{-3}	(calc6) (28)	47x10^3 11.22x10^4	(6) (16)	4.67 5.05	(6) (16)
pentachlorobenzene $C_6H .Cl_5$	250.36	0.135 0.560 1.3319 0.8312	(6) (16,24) (23) (20)	5.82x10^{-3} 3x10^{-3}	(calc6) (calc5)	15.4x10^4	(6,16)	5.19	(6)
Hexachlorobenzene C_6H_6	284.81	0.035 4.95x10^{-3} 5x10^{-3} 4.7x10^{-3}	(6,25) (16,24) (7,21) (20)	11x10^{-5} 2.91x10^{-3} 2.1x10^{-5}	(calc5) (Calc6) (7)	16,8x10^4 1.5x10^6	(6) (7)	5.23 6.18	(6) (35)

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	Log Kow	Ref
TOLUENE FAMILY									
Toluene	92.141	515	(7,13,19)	28.47	(22)	489.77	(calc7)	2.69	(17,19,26)
(methyl Benzene)		627	22	28.12	(28)	490	(7)		(calc7)
		470	(17,25)	30	(25)				
$C_6H_5.CH_3$		530	(22)	28.5	(13)				
		570	(12)	28.45	(calc2)				
		514.58	(26)	29.108	(calc5)				
		535.12	(26)	28.358	(calc6)				
		507.52	(26)						
		578.65	(20)						
o-Methyl Toluene	106.17	220.83	(20)	6.536	(28)	1318.3	(19)	3.12	(19)
(o-Xylene)		175	(19)			1348.9	(20)	3.13	(20)
$CH_3.C_6H_4.CH_3$									
m-Methyl Toluene	106.17	160.32	(20)	8.284	(28)	1584.9	(20)	3.20	(20)
(m-Xylene)		196	(22)						
$CH_3.C_6H_4.CH_3$		173	(22)						
p-Methyl Toluene	106.17	214.46	(20)	8.74	(28)	1513.6	(20)	3.18	(20)
(p-Xylene)		198	(22)						
$CH_3.C_6H_4.CH_3$		200	(22)						

TABLE A.2.1 - Continued...

COMPOUND	MW	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
o-Hydroxytoluene (o-cresol) (o-methyl phenol) $CH_3.C_6H_4.OH$	108.14	2.50×10^4	(8.15)	0.394	(calc6)	89.125	(37)	1.95	(37)
m-Hydroxytoluene (m-cresol) (m-methyl phenol) $CH_3.C_6H_4.OH$	108.14	2.60×10^4 0.50×10^4	(15) (8)	0.1199	(calc6)	104.71	(calc7)	2.02	(calc7)
p-Hydroxytoluene (p-cresol) (p-methyl phenol) $CH_3.C_6H_4.OH$	108.14	1.80×10^4 2.30×10^4	(1,8) (15)	0.1055 0.108	(calc6) (1)	87.096 158.49	(calc7) (1)	1.94 2.2	(calc7) (1)
o-Aminotoluene (o-Toluidine) (o-methylaniline) $CH_3.C_6.H_4.NH_2$	107.16	1.70×10^4 1.50×10^4	(15) (8)	0.249 0.265	(calc6) (calc2)	19.498	(37)	1.29	(37)
m-Aminotoluene (m-Toluidine) (m-methylaniline $CH_3.C_6H_4.NH_2$	107.16	25302	(calc1)	0.336 0.22	(calc6) (calc2)	25.119	(calc7)	1.4	(calc7)

TABLE A.2.1 - Continued...

COMPOUND	MW (g/mole)	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
p-Aminotoluene (p-Toluidine) (p-methylaniline) $CH_3.C_6H_4.NH_2$	107.16	0.70×10^4 0.74×10^4	(15) (8)	0.3025 0.3013	(calc6) (calc2)	24.547	(calc7)	1.39	(calc7)
o-Nitrotoluene (o-Methylnitrobenzene) $CH_3.C_6H_4.NO_2$	137.14	652 650(30°)	(14) (8)	0.195	(calc6)	199.53	(37)	2.30	(37)
m-Nitrotoluene (m-Methylnitrobenzene) $CH_3.C_6H_4.NO_2$	137.14	498 500(30°)	(14) (8)	0.2093	(calc6)	263.03	(calc7)	2.42	(calc7)
p-Nitrotoluene (p-Methylnitrobenzene) $CH_3.C_6H_4.NO_2$	137.14	442	(14)	0.17	(calc6)	234.42	(calc7)	2.37	(calc7)

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S g/m^3	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
PHENOL FAMILY									
Phenol	94.11	$8.66x10^4$	(13)	0.2948	(calc6)	29	(7)	1.46	(calc7)
(Carbolic acid)		$9.30x10^4$	(15)	0.3513	(calc2)				
(Benzenol)		$8.20x10^4$ (15°)	(8)	0.41	(13)				
(Hydroxybenzene)		$8.20x10^4$	(6)						
$C_6H_5.OH$									
o-Chlorophenol	128.56	$2.90x10^4$	(18)	2.295	(calc6)	141.25	(calc7)	2.15	(calc7)
$HO.C_6H_4.Cl$		$2.80x10^4$	(15)					2.2	(18)
		$2.85x10^4$ (20°)	(8)						
		$1.14x10^4$	(23)						
m-chlorophenol	128.56	$2.60x10^4$	(15)	0.276	(calc6)	316.23	(calc7)	2.5	(calc7)
$HO.C_6H_4.Cl$		$2.60x10^4$ (20°)	(8)						
p-chlorophenol	128.56	$2.70x10^4$	(15)	0.19	(calc6)	245.47	(calc7)	2.39	(calc7)
$HO.C_6H_4.Cl$		$2.71x10^4$ (20°)	(8)						

TABLE A.2.1 - Continued...

COMPOUND	MW (g/mole)	S (g/m^3)	Ref	P (mm Hg)	Ref	Kow	Ref	Log Kow	Ref
o-Methyl phenol (o-Cresol) $CH_3.C_6H_4.OH$	108.14	$2.50x10^4$ $2.50x10^4$	(8) (15)	0.394	(calc6)	89.125	(37)	1.95	(37)
m-Methyl phenol (m-Cresol) (m-Hydroxytoluene) $CH_3.C_6H_4.OH$	108.14	$2.60x10^4$ $2.50x10^4$ $0.50x10^4$	(15) (8)	0.1199	(calc6)	104.71	(calc7)	2.02	(calc7)
p-Methyl phenol (p-Cresol) (p-Hydroxytoluene) $Ch_3.C_6H_4.OH$	108.14	$1.80x10^4$ $1.80x10^4$ $2.30x10^4$	(8) (1) (15)	0.1055 0.108	(calc6) (1)	87.-96 158.49	(calc7) (1)	1.94 2.2	(calc7) (1)
m-Ethyl phenol $C_2H_5.C_6H_4.OH$	122.17	928.03	(calc1)	0.079	(calc6)	251.19	(calc7)	2.4	(calc7)

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S (g/m^3)	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
o-Hydroxyphenol (Catechol) (Pyrocatechol)	110.11	45.1x10^4	(8)	0.0328	(calc6)	7.5858	(37)	0.88	(37)
(pyrocatechin) (1,2-dihydroxy-benzene)		45x10^4	(15)						
HO.C$_6$H$_4$-OH									
m-Hydroxyphenol	110.11	147.3x10^4 (12.5 °C)	(8)	1.92x10^{-3}	(calc6)	6.3096	(calc7)	0.8	(calc7)
(Resorcinol)									
(1,3 dihydroxy-benzene)		123x10^4	(15)						
HO.C$_6$H$_4$.OH									
p-Hydroxyphenol (hydroquinone) (Quinol) (1,4 dihydroxy-benzene)	110.11	8x10^4 6x10^4(15°)	(15) (8)	7.29x10^{-6}	(calc6)	3.8905	(calc7)	0.59	(calc7)
HO.C$_6$H$_4$.OH									
o-Nitrophenol	139.11	1.35x10^4(20°) 0.2x10^4	(8) (15)	0.1884	(calc6)	61.66	(calc7)	1.79	(calc7)
HO.C$_6$H$_4$.NO$_2$		0.21x10^4	(7)			61.66	(7)		

COMPOUND	MW g/mole	S (g/cm^3)	Ref	P (mm Hg)	Ref	Kow	Ref	log Kow	Ref
<u>ANILINE FAMILY</u>									
Aniline (Aminobenzene) $C_6H_5.NH_2$	93.13	$3.66x10^4$ $3.38x10^4$ $3.70x10^4$ $3.60x10^4 (18^o)$ $3.66x10^4$	(6) (13) (15) (8) (7)	0.4685 0.6252	(calc6) (calc2)	7.9433 9.5	(calc7) (7)	0.9	(calc7)
o-Chloroaniline $NH_2.C_6H_4.Cl$	127.58	8760	(13)	0.217 0.254 0.253	(calc6) (calc2) (13)	79.433	(37)	1.90	(37)
m-Chloroaniline $NH_2.C_6H_4.Cl$	127.58	5787.6	calc1	0.0572 0.0829	(calc6) (calc2)	75.858	(calc7)	1.88	(calc7)
p-Chloroaniline $NH_2.C_6H_4.Cl$	127.58	3900 6872.6 3000	21 calc1 (7)	0.0966 0.0248	(calc6) (21)	68	(7)	1.83	(calc7)

TABLE A.2.1 - Continued...

COMPOUND	MW (g/mole)	S (g/m^3)	Ref	P mm Hg	Ref	Kow	Ref	log Kow	Ref
o-methylaniline (o-Toludine) (o-Amino toluene) $NH_2.C_6H_4.CH_3$	107.16	1.70×10^4 1.50×10^4	(15) (8)	0.249 0.265	(calc6) (calc2)	19.498	(37)	1.29	(37)
m-methylaniline (m-Toludine) (m-Aminotoluene) $NH_2.C_6H_4.CH_3$	107.16	25302	(calc1)	0.336 0.22	(calc6) (calc2)	25.119	(calc7)	1.4	(calc7)
p-methylaniline (p-Toluidine) (p-Aminotoluene) $NH_2.C_6H_4.CH_3$	107.16	0.70×10^4 0.74×10^4 (21°)	(15) (8)	0.3025 0.3013	(calc6) (calc2)	24.547	(calc7)	1.39	(calc7)
m-Phenylenediamine (m-Diaminobenzene) $NH_2.C_6H_4.NH_2$	108.15	25×10^4	(15)	5.52×10^{-3}	(calc6)	5.445	(calc9)	0.736	(calc9)

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S g/m^3	Ref	P (mm Hg)	Ref	Kow	Ref	log Kow	Ref
o-Nitroaniline (o-nitraline) (n-aminonitro-benzene) $NO_2.C_6H_4.NH_2$	138.13	1212 1000 (1470(30°)	(14) (15) (14)	$4.09x10^{-3}$	(calc6)	229.09	(calc9)	2.36	(calc9)
m-Nitroaniline (m-nitraniline) (m-aminonitro-benzene $NO_2.C_6H_4.NH_2$	138.13	1210 910 $0.1x10^4$ $0.11x10^4$	(14) (14) (15) (8)	$1.22x10^{-3}$	(calc6)	23.442	(calc7)	1.37	(calc7)
p-Nitroaniline (p - Nitraniline) (p-Aminonitro-benzene) $NO_2.C_6H_4.NH_2$	138.13	$0.08x10^4$ (18.5°) $0.05x10^4$ 7.28 $0.08-222x10^4$	(8) (15) (12) (27)	$2.99x10^4$	(calc6)	24.547	(calc7)	1.39	(calc7)

TABLE A.2.1 - Continued...

COMPOUND	MW g/mole	S g/m^3	Ref.	P mm Hg	Ref.	Kow	Ref	log Kow	Ref.
NITROBENZENE FAMILY									
Nitrobenzene $C_6H_5.NO_2$	123.11	2050 1780 $0.19x10^4$ (20°)	(14) (6) (8)	0.265	(calc6)	70.795 62	(calc7) (6)	1.85 1.792	(calc7) (6)
o-methylnitrobenzene (o-nitrotoluene) $NO_2.C_6H_4.CH_3$	137.14	652 650	(14) (8)	0.195	(calc6)	199.53	(37)	2.30	(37)
m-methylnitrobenzene (m-nitrotoluene) $NO_2.C_6H_4.CH_3$	137.14	498 500(30°)	(14) (8)	0.2093	(calc6)	263.03	(calc7)	2.42	(calc7)
p-methylnitrobenzene (p-nitrotoluene) $NO_2.C_6H_4.CH_3$	137.14	442	(14)	0.17	(calc6)	234.43	(calc7)	2.37	(calc7)

COMPOUND	mw	S (g/m^3)	Ref	p (mm Hg)	Ref	Kow	Ref	log Kow	Ref
o-Hydroxynitrobenzene $NO_2.C_6H_4.OH$	139.11	$0.2\text{x}10^4$ $0.21\text{x}10^4$	(15) (8)	0.188	(calc6)	61.66	(calc7)	1.79	(calc7)
o-Aminonitrobenzene $NO_2.C_6H_4.NH_2$	138.13	1212	(14)	$4.09\text{x}10^{-3}$	(calc6)	229.09	(calc9)	2.36	(calc9)
m-Aminonitrobenzene $NO_2.C_6H_4.NH_2$	138.13	1100(20°) 1210 910	(8) (14) (14)	$1.22\text{x}10^{-3}$	(calc6)	23.442	(calc7)	1.37	(calc7)
p-Aminonitrobenzene $NO_2.C_6H_4.NH_2$	138.13	$0.08\text{x}10^4$ (18.5°) 728 $0.05\text{x}10^4$ $0.08\text{-}2.22\text{x}10^4$	(8) (12) (15) (27)	$2.99\text{x}10^{-4}$	(calc6)	24.547	(calc7)	1.39	(calc7)

TABLE A.2.2 The Antoine Constants

NAME OF CHEMICAL	A	B	C	Range ^oC	Ref
MONOSUBSTITUTED BENZENE FAMILY					
Benzene	6.9057	1211.03	220.79		(30)
	6.8927	1203.53	219.88		(31)
Fluorobenzene	7.1870	1381.83	235.56		(31)
Chlorobenzene	7.1069	1500.00	224.00	0 to 42	(30)
Bromobenzene	6.8834	1440.1	204.00		(30)
Iodobenzene	6.8951	1562.87	201.00		(30)
Methylbenzene	6.9546	1344.80	219.48		(30)
Benzylalcohol	7.8184	1950.30	194.36	20 to 113	(30)
Acetophenone	(eq 2.13)	55.1170	9.1352	30 to 100	(30)
Phenol	7.1362	1518.10	175.00		(30)
Anisole	6.9893	1453.80	200.00		(30)
Aniline	7.2418	1675.30	200.00		(30)

TABLE A.2.2 Continued

NAME OF CHEMICAL	A	B	C	Range	Ref
HALOBENZENE FAMILY					
Fluorobenzene	7.1870	1381.83	235.56		(31)
Chlorobenzene	7.1069	1500.00	224.00	0 to 42	(30)
	6.9781	1431.05	217.55		(31)
Bromobenzene	6.8834	1440.10	204.00		(30)
	6.8600	1438.82	205.44		(31)
Iodobenzene	6.8951	1562.87	201.00		(30)
	7.0119	1640.12	208.77		(31)
o-dichlorobenzene	7.1438	1704.49	219.42		(31)
m-dichlorobenzene	7.0401	1607.05	213.38		(31)
p-dichlorobenzene	6.8980	1507.30	201.00		(30)
	7.0208	1590.88	210.23		(31)
o-dibromobenzene	7.5013	2093.70	230.00		(30)

TABLE A.2.2 Continued

NAME OF CHEMICAL	A	B	C	Range ^oC	Ref
PHENOL FAMILY					
Phenol	7.1362	1518.10	175.0		(30)
o-chlorophenol	7.242	1668.00	210.0	18 to 80	(30)
ANILINE FAMILY					
Aniline	7.2418	1675.30	200.0		(30)
o-chloroaniline	7.5627	1998.60	220.0	20 to 108	(30)
m-chloroaniline	7.5594	2073.75	215.0	15 to 125	(30)
o-methylaniline	7.2258	1728.17	202.0		(30)
m-methylaniline	7.3900	1810.80	200.0	20 to 105	(30)
p-methylaniline	7.2602	1758.55	201.0		(30)

TABLE A.2.3. Melting Points and Boiling Points for Halogenated benzenes

NAME OF CHEMICAL	t_m °C	Ref	t_b °C	Ref
HALOBENZENE FAMILY				
Benzene	5.5	(9)	80.1	(9)
Fluorobenzene	-41.2	(9)	85.1	(9)
Chlorobenzene	-45.6	(9)	132	(9)
Bromobenzene	-30.82	(9)	156	(9)
Iodobenzene	-31.27	(9)	188.3	(9)
o-difluorobenzene	-34	(9)	92	(15)
m-difluorobenzene	-59	(9)	83	(15)
p-difluorobenzene	-13	(9)	89	(15)
o-dichlorobenzene	-17	(9)	180.5	(9)
m-dichlorobenzene	-24.7	(9)	173	(9)
p-dichlorobenzene	53	(9,16)	174	(9)
o-dibromobenzene	77.1	(9)	225	(9)
m-dibromobenzene	-7	(9)	218	(9)
p-dibromobenzene	87	(9,16)	219	(9)
o-diiodobenzene	27	(9,16)	286	(9)
m-diiodobenzene	40	(9,16)	285	(9)
p-diiodobenzene	132	(9,16)	285 sub.	(9)
o-bromochlorobenzene	-12.3	(9)	204	(9)
m-bromochlorobenzene	-21.5	(9)	196	(9)
p-bromochlorobenzene	68	(9)	196	(9)
p-bromoiodobenzene	92	(9,16)	$252^{754\ \text{mm}}$	(9)

TABLE A.2.3 Continued

NAME OF CHEMICAL	t_m ^oC	Ref	t_b ^oC	Ref
o-chlorolodobenzene	$<25^0$	(16)	234.5	(9)
m-chlorolodobenzene	$<25^0$	(16)	230	(9)
p-chlorolodobenzene	57	(9,16)	227	(9)
1,2,3-trichlorobenzene	53	(9,16)	218	(9)
1,2,4-trichlorobenzene	16.95	(9)	213.5	(9)
1,3,5-trichlorobenzene	63	(9,16)	208	(9)
1,2,4-tribromobenzene	44	(9,16)	275	(9)
1,3,5-tribromobenzene	122	(9,16)	271	(9)
1,2,3,4-tetrachlorobenzene	47.5	(9,16)	254	(9)
1,2,3,5-tetrachlorobenzene	54.5	(9,16)	246	(9)
1,2,4,5-tetrachlorobenzene	140	(9,16)	245	(9)
Pentachlorobenzene	86	(9,16)	277	(9)
Hexachlorobenzene	284.79	(9,16)	322 sub.	(9)

TABLE A.2.4 The vapor pressure-temperature data for several classes of substituted benzenes taken from list of Stull D.R. [34]

NAME OF CHEMICAL	P_1 mmHg	t_1 °C	P_2 mmHg	t_2 °C	P_3 mmHg	t_3 °C
MONOSUBSTITUTED BENZENE FAMILY						
Benzene	60	15.4	X	25	100	26.1
Fluorobenzene	60	19.6	X	25	100	30.4
Chlorobenzene	10	22.2	X	25	20	35.3
Bromobenzene	X	25	5	27.8	10	40
Iodobenzene	1	24.1	X	25	5	50.6
Toluene	20	18.4	X	25	40	31.8
Butylbenzene	1	22.7	X	25	5	48.8
Benzylalcohol	X	25	1	58.0	5	80.8
Phenol	X	25	5	62.5	10	73.8
Aniline	X	25	1	34.8	5	57.9
Nitrobenzene	X	25	1	44.4	5	71.6
HALOBENZENE FAMILY						
Fluorobenzene	60	19.6	X	25	100	30.4
Chlorobenzene	10	22.2	X	25	20	35.3
Bromobenzene	X	25	5	27.8	10	40
Iodobenzene	1	24.1	X	25	5	50.6
o-dichlorobenzene	1	20	X	25	5	46.0
m-dichlorobenzene	1	12.1	X	25	5	39.0
p-dichlorobenzene	X	25	10	54.8	20	69.2
p-bromochlorobenzene	X	25	1	32	5	59.5
1,2,3-trichlorobenzene	X	25	1	40	5	70.0

TABLE A.2.4 Continued

NAME OF CHEMICAL	P_1 mmHg	t_1 ^oC	P_2 mmHg	t_2 ^oC	P_3 mmHg	t_3 ^oC
1,2,4-trichlorobenzene	X	25	1	38.4	5	67.3
1,3,5-trichlorobenzene	X	25	5	63.8	10	81.7
1,2,3,4-tetrachlorobenzene	X	25	1	68.5	5	99.6
1,2,3,5-tetrachlorobenzene	X	25	1	58.2	5	89.0
1,2,4,5-tetrachlorobenzene	X	25	40	146.0	60	157.7
Pentachlorobenzene	X	25	1	98.6	5	129.7
Hexachlorobenzene	X	25	1	114.4	5	149.3
PHENOL FAMILY						
Phenol	X	25	5	62.5	10	73.8
o-chlorophenol	1	12.1	X	25	5	38.2
m-chlorophenol	X	25	1	44.2	5	72.0
p-chlorophenol	X	25	1	49.8	5	78.2
o-methylphenol	X	25	1	38.2	5	64.0
m-methylphenol	X	25	1	52.0	5	76.0
p-methylphenol	X	25	1	53.0	5	76.5
m-ethylphenol	X	25	1	60.0	5	86.8
o-hydroxyphenol	X	25	5	104	10	118.3
m-hydroxyphenol	X	25	1	108	5	138.0
o-nitrophenol	X	25	1	49.3	5	76.8
ANILINE FAMILY						
Aniline	X	25	1	34.8	5	57.9

TABLE A.2.4. Continued

NAME OF CHEMICAL	P_1 mmHg	t_1 ^oC	P_2 mmHg	t_2 ^oC	P_3 mmHg	t_3 ^oC
o-chloroaniline	X	25	1	46.3	5	72.3
m-chloroaniline	X	25	1	63.5	5	89.8
p-chloroaniline	X	25	1	59.3	5	87.9
o-methylaniline	X	25	1	44.0	5	69.3
m-methylaniline	X	25	1	41.0	5	68.0
p-methylaniline	X	25	1	42.0	5	68.2
m-phenylenediamine	X	25	1	99.8	5	131.2
o-nitroaniline	X	25	1	104.0	5	135.7
m-nitroaniline	X	25	1	119.3	5	151.5
p-nitroaniline	X	25	1	142.4	5	177.6
N,N dimethylaniline	X	25	1	29.5	5	56.3
NITROBENZENE FAMILY						
Nitrobenzene	X	25	1	44.4	5	71.6
o-methylnitrobenzene	X	25	1	50.0	5	79.1
m-methylnitrobenzene	X	25	1	50.2	5	81.0
p-methylnitrobenzene	X	25	1	53.7	5	85.0
o-hydroxynitrobenzene	X	25	1	49.3	5	76.8
o-aminonitrobenzene	X	25	1	104.0	5	135.7
m-aminonitrobenzene	X	25	1	119.3	5	151.5
p-aminonitrobenzene	X	25	1	142.4	5	177.6

TABLE A.2.5 π Substituent Constant Values derived from four different systems taken from list of Fujita[36]

Function	Phenols	Anilines	Nitrobenzenes	Benzenes
H	0	0	0	0
2-F	0.25 ± 0.01			
3-F	0.47 ± 0.01	0.40 ± 0.02		0.14 ± 0.02
4-F	0.31 ± 0.01	0.25 ± 0.02		
2-CL	0.69 ± 0.01			
3-Cl	1.04 ± 0.01	0.98 ± 0.02	0.61 ± 0.03	0.71 ± 0.03
4-Cl	0.93 ± 0.01		0.54 ± 0.03	
2-Br	0.89 ± 0.01			
3-Br	1.17 ± 0.01		0.79 ± 0.03	0.86 ± 0.02
4-Br	1.13 ± 0.01			
2-I	1.19 + 0.01			
3-I	1.47 ± 0.01			
4-I	1.45 ± 0.01			
2-CH_3				
3-CH_3	0.56 ± 0.01	0.50 ± 0.02	0.57 ± 0.03	0.56 ± 0.02
4-CH_3	0.48 ± 0.01	0.49 ± 0.02	0.52 ± 0.02	

TABLE A.2.5 Continued

Function	Phenols	Anilines	Nitrobenzenes	Benzenes
3-Et	0.94 ± 0.01			
3-CH_2OH	-1.02 ± 0.03	-0.95 ± 0.02	-0.65 ± 0.02	-1.03 ± 0.02
4-CH_2OH	-1.26 ± 0.05		-0.60 ± 0.02	
3-$COCH_3$	-0.07 ± 0.01		-0.43 ± 0.02	0.55 ± 0.02
4-$COCH_3$	-0.11 ± 0.01		-0.36 ± 0.02	
2-OH				
3-OH	-0.66 ± 0.01	-0.73 ± 0.04	0.15 ± 0.03	0.67 ± 0.01
4-OH	-0.87 ± 0.03	-1.07 ± 0.02	0.11 ± 0.03	
3-OCH_3	0.12 ± 0.01	0.03 ± 0.02	0.31 ± 0.02	-0.02 ± 0.02
4-OCH_3	0.12 ± 0.01		0.18 ± 0.02	
3-NH_2	-1.29 ± 0.03		-0.48 ± 0.02	-1.23 ± 0.02
4-NH_2	-1.63 ± 0.02		-0.46 ± 0.02	
3-$N(CH_3)_2$	0.10 ± 0.01			0.18 ± 0.02
2-NO_2	0.33 ± 0.01	0.47 ± 0.02		
3-NO_2	0.54 ± 0.02	0.49 ± 0.02	-0.36 ± 0.02	-0.28 ± 0.02
4-NO_2	0.50 ± 0.01		-0.39 ± 0.02	

The following values for log Kow enable one to calculate Kow for any of the compounds listed in this table, Phenol 1.46 ± 0.01, Aniline 0.90 ± 0.01, Nitrobenzene 1.85 ± 0.01, Benzene 2.13 ± 0.1

TABLE A.2.6 Aromatic *f* values taken from list of Rekker[37]

FRAGMENT	*f*
F	0.412
Cl	0.943
Br	1.168
I	1.460
OH	-0.359
NH_2	-0.897
NO_2	-0.077
C_6H_5	1.90

TABLE A.2.7 Input Data Used for Calculations

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/GMOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref.	P VAPOUR PRESSURE (mmHg)	Ref	log K_{OW} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
<u>MONOSUBSTITUTED BENZENE FAMILY</u>							
Benzene	78.114	1790	(7,22)	95.044	(calc 4, calc 6)	2.13	(17,19,26)
Fluorobenzene	96.106	1553	(19)	77.819	(calc 6)	2.27	(17,calc 7)
Chlorobenzene	112.56	480	(1)	11.656	(calc 6)	2.84	(17,calc 8)
Bromobenzene	157.02	410.6	(19)	4.2286	(calc 6)	2.99	(17,calc 7)
Iodobenzene	204.01	340	(14,17,19)	1.0611	(calc 6)	3.36	(16)
Toluene	106.17	470	(17,25)	28.358	(calc 6)	2.69	(17,19,26 calc7)
Ethyl benzene	106.17	152	(13,19)	9.6	(13)	3.15	(19,26,37)
n-Propyl benzene	120.20	55	(19)	3.4276	(28)	3.68	(19,26)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/GMOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOUR PRESSURE (mmHg)	Ref	log Kow LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
Iscpropyl benzene	120.20	50	(13.19)	4.6	(13)	3.66	(19,26,37)
Butyl benzene	134.22	5000	(13)	1.1	(13)	1.94	(calc 9)
Benzyl alcohol (Phenyl carbinol) (α Hydroxy toluene)	108.14	$4x10^4$	(18,25)	0.06	(calc 6)	1.1	(calc 7)
Acetophenone (Acetyl benzene) (Methylphenylketone)	120.15	$15.3x10^3$	(calc 1)	0.3021	(calc 3)	1.58	(calc 7)
Phenol (Hydroxy benzene) (carbolic acid) (Benzenol)	94.11	$9.3x10^4$	(15)	0.2948	(calc 6)	1.46	(calc 7)
Anisole (Methylphenylether)	108.14	$1.04x10^4$	(13)	3.372	(calc 2)	2.11	(calc 7)
Aniline (Amino benzene)	93.13	$3.66x10^4$	(6)	0.4685	(calc 6)	0.9	(calc 7)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/GMOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref.	P VAPOR PRESSURE (mmHg)	Ref	log K_{OW} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
N,N-Dimethylaniline	121.18	1.25×10^3	(calc 1)	0.7418	(calc 6)	2.31	(calc 7)
Nitrobenzene	123.11	2050	(12)	0.265	(calc 6)	1.85	(calc 7)
HALOBENZENE FAMILY							
Fluorobenzene	96.116	1553	(19)	77.819	(calc 6)	2.27	(17,calc 7)
Chlorobenzene	112.56	480	(1)	11.656	(calc 6)	2.84	(17)
Bromobenzene	157.02	410.6	(19)	4.2286	(calc 6)	2.99	(17)
Iodobenzene	204.01	340	(14,17,19)	1.0611	(calc 6)	3.36	(16)
o-Difluorobenzene	114.09	1140.9	(16,24)	62.596	(calc 5)	2.59	(16)
m-Difluorobenzene	114.09	1140.9	(16,24)	89.66	(calc 5)	2.58	(16)
p-Difluorobenzene	114.09	1224.4	(16,24)	70.614	(calc 5)	2.58	(16)
o-Dichlorobenzene	147.01	150	(18)	1.3928	(calc 6)	3.59	(16)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/GMOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOR PRESSURE (mmHg)	Ref	log K_{OW} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
m-Dichlorobenzene	147.01	120	(18)	2.2435	(calc 6)	3.59	(16)
p-Dichlorobenzene	147.01	791	(1,6,17, 18,25)	1.9261	(calc 6)	3.39	(6,17)
o-Dibromobenzene	235.92	74.6	(16,24)	0.1953	(calc 2)	4.07	(16)
m-Dibromobenzene	235.92	98.347	(16,24)	0.2261	(calc 5)	4.07	(16)
p-Dibromobenzene	235.92	20.08	(16,24)	0.1611	(28)	4.07	(16)
o-Diiodobenzene	329.91	18.984	(16,24)	7.26×10^{-3}	(calc 5)	4.65	(16)
m-Diiodobenzene	329.91	8.8796	(16,24)	5.68×10^{-3}	(calc 5)	4.64	(16)
p-Diiodobenzene	329.91	1.855	(16,24)	6.97×10^{-4}	(calc 5)	4.64	(16)
o-Bromochlorobenzene	191.46	123.62	(16,24)	0.4425	(calc 5)	3.83	(16)
m-Bromochlorobenzene	191.46	118.5	(16,24)	0.6465	(calc 5)	3.83	(16)
p-Bromochlorobenzene	191.46	44.882	(16,24)	0.6331	(calc 6)	3.83	(16)
p-Bromoiodobenzene	282.91	7.7919	(16)	9.23×10^{-3}	(calc 5)	4.36	(16)
o-Chloroiodobenzene	238.46	68.773	(16,24)	0.1012	(calc 5)	4.12	(16)
m-Chloroiodobenzene	238.46	67.207	(16)	0.1262	(calc 5)	4.12	(16)
p-Chloroiodobenzene	238.46	22.254	(16,24)	7.04×10^{-2}	(calc 5)	4.12	(16)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/G MOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOUR PRESSURE (mmHg)	Ref	Log K_{OW} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
1,2,3-Trichlorobenzene	181.46	31.532	(16)	0.3961	(calc 6)	4.27	(16)
1,2,4-Trichlorobenzene	181.46	30	(6,7)	0.4265	(calc 6)	4.18	(calc 7)
1,3,5-Trichlorobenzene	181.46	6.588	(16)	0.8363	(calc 6)	4.27	(16)
1,2,4-Tribromobenzene	314.82	9.955	(16)	8.65×10^{-3}	(calc 5)	4.98	(16)
1,3,5-Tribromobenzene	314.82	0.79	(16)	1.79×10^{-3}	(calc 5)	4.98	(16)
1,2,3,4-Tetrachlorobenzene	215.91	4.307	(16)	0.0599	(calc 6)	5.05	(16)
1,2,3,5-Tetrachlorobenzene	215.91	3.5	(16)	0.2116	(calc 6)	5.05	(16)
1,2,4,5-Tetrachlorobenzene	215.91	6	(6)	0.093	(calc 6)	4.67	(6)
Pentachlorobenzene	250.36	0.135	(6)	5.82×10^{-3}	(calc 6)	5.19	(6)
Hexachlorobenzene	284.81	5×10^{-3}	(7,21)	2.1×10^{-5}	(7)	5.23	(6)
<u>TOLUENE FAMILY</u>							
Toluene	92.14	470	(17,25)	28.358	(calc 6)	2.69	(17,19,26 calc 7)
o-Xylene (o-methyl toluene)	106.17	175	(19)	6.536	(28)	3.12	(19)
m-Xylene (m-methyl toluene)	106.17	160.32	(20)	8.284	(28)	3.20	(20)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/G MOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOR PRESSURE (mmHg)	Ref	log K_{ow} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
p-Xylene (p-Methyltoluene)	106.17	214.46	(20)	8.74	(28)	3.18	(20)
o-Cresol (o-Hydroxytoluene) (o-Methyl phenol)	108.14	$2.50\text{x}10^4$	(8,15)	0.394	(calc 6)	1.95	(37)
m-Cresol (m-Hydroxytoluene (m-methyl phenol)	108.14	$0.50\text{x}10^4$	(8)	0.1199	(calc 6)	2.02	(calc 7)
p-Cresol (p-Hydroxytoluene) (p-methyl phenol)	108.14	$1.80\text{x}10^4$	(1,8)	0.1055	(calc 6)	1.94	(calc 7)
o-Toluidine (o-Aminotoluene) (o-Methylaniline)	107.16	$1.50\text{x}10^4$	(8)	0.249	(calc 6)	1.29	(37)
m-Toluidine (m-Aminotoluene) (m-methyloniline)	107.16	25302	(calc 1)	0.336	(calc 6)	1.4	(calc 7)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/G MOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOUR PRESSURE (mmHg)	Ref	log K_{OW} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
p-Toluidine (p-Aminotoluene) (p-methylaniline)	107.16	0.74×10^4	(8)	0.3025	(calc 6)	1.39	(calc 7)
o-Nitrotoluene (o-Methylnitrobenzene)	137.14	650	(8)	0.195	(calc 6)	2.30	(37)
m-Nitrolutoluene (m-Methylnitrobenzene)	137.14	498	(14)	0.2093	(calc 6)	2.42	(calc 7)
p-Nitrotoluene (p-Methylnitrobenzene)	137.14	442	(14)	0.17	(calc 6)	2.37	(calc 7)
PHENOL FAMILY							
Phenol (Carbolic-acid) (Benzenol) (Hydroxybenzene)	94.11	8.66×10^4	(13)	0.2948	(calc 6)	1.46	(calc 7)
o-chloro phenol	128.56	2.90×10^4	(18)	2.295	(calc 6)	2.15	(calc 7)
m-chloro phenol	128.56	2.60×10^4	(15)	0.276	(calc 6)	2.5	(calc 7)
p-chlorophenol	128.56	2.70×10^4	(15)	0.19	(calc 6)	2.39	(calc 7)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/G MOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOUR PRESSURE (mm Hg)	Ref	Log K_{ow} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
o-Cresol (o-Methylphenol) (o-Hydroxytoluene)	108.14	2.50×10^4	(8,15)	0.394	(calc 6)	1.95	(37)
m-Cresol (m-methylphenol) (m-Hydroxyltoluene)	108.14	0.50×10^4	(8)	0.1199	(calc 6)	2.02	(calc 7)
p-Cresol (p-methylphenol) (p-Hydroxytoluene)	108.14	1.80×10^4	(1,8)	0.1055	(calc 6)	1.94	(calc 7)
m-ethyl phenol	122.17	928.03	(calc 1)	0.079	(calc 6)	2.4	(calc 7)
Catechol (o-Hydroxyphenol) (o-Dihydroxybenzene) (Pyrocatechol) (Pyrocatechin)	110.11	45.1×10^4	(8)	0.0328	(calc 6)	0.88	(37)
Resorcinol (m-Hydroxyphenol) (m-Dihydroxybenzene)	110.11	147.3×10^4	(8)	1.92×10^{-3}	(calc 6)	0.8	(calc 7)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/G MOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOUR PRESSURE (mmHg)	Ref	log K_{ow} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
Hydroquinone (p-Hydroxyphenol) (p-Dihydroxybenzene) (Quinol)	110.11	$8x10^4$	(15)	$7.29x10^{-6}$	(calc 6)	0.59	(calc 7)
o-Nitrophenol	139.11	$1.35x10^4$	(8)	0.1884	(calc 6)	1.79	(calc 7)
ANILINE FAMILY							
Aniline (Aminobenzene)	93.13	$3.66x10^4$	(6.7)	0.4685	(calc 6)	0.9	(calc 7)
o-Chloroaniline	127.58	8760	(13)	0.254	(calc 2)	1.90	(37)
m-Chloroaniline	127.58	5787.6	(calc 1)	0.0572	(calc 6)	1.88	(calc 7)
p-Chloroaniline	127.58	3900	(21)	0.0248	(21)	1.83	(calc 7)
o-Toluidine (o-Methylaniline) (o-Aminotoluene)	107.16	$1.50x10^4$	(8)	0.249	(calc 6)	1.29	(37)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/G MOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOUR PRESSURE (mmHg)	Ref	Log K_{OW} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
m-Toluidine (m-Methylaniline) (m-Amino toluene)	107.16	25302	(calc 1)	0.336	(calc 6)	1.4	(calc 7)
p-Toluidine (p-Methylaniline) (p-Aminotoluene)	107.16	0.70×10^4	(15)	0.3025	(calc 6)	1.39	(calc 7)
m-Phenylenediamine (m-Diaminobenzene)	108.15	25×10^4	(15)	5.52×10^{-3}	(calc 6)	0.736	(calc 9)
o-Nitroaniline (o-Nitraniline) (o-Aminonitrobenzene)	138.13	1212	(14)	4.09×10^{-3}	(calc 6)	2.36	(calc 9)
m-Nitroaniline (m-Nitraniline) (m-Aminonitro-benzene)	138.13	1210	(14)	1.22×10^{-3}	(calc 6)	1.37	(calc 7)
p-Nitroaniline (p-Nitraniline) (p-Aminonitro-benzene	138.13	2.22×10^4	(27)	2.99×10^{-4}	(calc 6)	1.39	(calc 7)

TABLE A.2.7 Continued

NAME OF CHEMICAL	MW MOLECULAR WEIGHT (G/G MOLE)	S AQUEOUS SOLUBILITY (PPM)	Ref	P VAPOUR PRESSURE (mmHg)	Ref	Log K_{ow} LOG OF OCTANOL WATER PARTITION COEFFICIENT	Ref
<u>NITROBENZENE FAMILY</u>							
Nitrobenzene	123.11	2050	(14)	0.265	(calc 6)	1.85	(Calc 7)
o-Methylnitrobenzene (o-Nitrotoluene)	137.14	650	(8)	0.195	(calc 6)	2.30	(37)
m-Methylnitrobenzene (m-Nitrotoluene)	137.14	498	(14)	0.2093	(calc 6)	2.42	(calc 7)
p-Methylnitrobenzene (p-Nitrotoluene)	137.14	442	(14)	0.17	(calc 6)	2.37	(calc 7)
o-Hydroxynitrobenzene (o-Nitrophenol)	139.11	0.21×10^4	(8)	0.188	(calc 6)	1.79	(calc 7)
o-Aminonitrobenzene (o-Nitroaniline) (o-Nitraniline)	138.13	1212	(14)	4.09×10^{-3}	(calc 6)	2.36	(calc 9)
m-Aminonitrobenzene (m-Nitroaniline) (m-Nitraniline)	138.13	1210	(14)	1.22×10^{-3}	(calc 6)	1.37	(calc 7)
p-Aminonitrobenzene (p-Nitroaniline) (p-Nitraniline)	138.13	2.22×10^4	(27)	2.99×10^{-4}	(calc 6)	1.39	(calc 7)

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