ENVIRONMENTAL DISTRIBUTION OF POLYCHLORINATED BIPHENYLS BY TOPOLOGY BASED CHARACTERISTIC ROOT INDEX

by

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To the Memory of My Father Mehmet Türker

and

To Mikail

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ABSTRACT

Relationships between a newly developed index -which is based on topological characteristics of the molecules and called the Characteristic Root (CR) index- and the environmentally relevant physicochemical properties of the Polychlorinated Biphenyls, namely, aqueous solubility, vapour pressure, Henry's Law Constants, and octanol-water partition coefficient are discussed.

Correlations performed on the congeners clearly demonstrate that the CR index model accurately predicts the physicochemical properties of PCBs. High correlation coefficient ($r = 0.998$) was calculated for the linear one-parameter correlation between the CR index and molecular total surface area. So, the CR index was used in the prediction of properties dependent on total surface area. The quality and reliability of the correlations are shown to be high enough for environmental applications.

Reported experimental physicochemical data of PCBs are tabulated. Recommended values are given for 58 of the 209 congeners. With the available data, it is possible to estimate what percentage of the chemical will be located in the soil, bottom sediments, water and air. The predicted and experimental physicochemical properties of PCBs were used to predict the environmental compartmentalization of these compounds in an evaluative environment using the fugacity approach.

ÖZET

Bu çalışmada, yeni türetilen ve karakteristik kök (CR) adı verilen bir indeks ile, çevre açısından önemli bir kirletici grubu teşkil eden Poliklorlu Bifeniller'in (PCBs) sudaki çözünürlükleri, buhar basınçları ve oktanol-su oranı katsayıları gibi fizikokimyasal özellikleri arasindaki ilişki araştırılmıştır.

Elde edilen sonuçlar, CR indeksinin, fizikokimyasal özelliklerin tahmin edilmesinde geçerli bir yapısal parametre olduğunu göstermiştir. Metod, yapısal çizit, moleküler topoloji ve yapı-etki ilişkilerine bağlı olarak geliştirilmiştir. Bu metodla, 58 Poliklorlu Bifenil'in, çevredeki dağılımlarının kontrol edilmesinde önemli rol oynayan fizikokimyasal özellikleri hesaplanmıştır.

Bu değerler, Mackay tarafından geliştirilen, maddenin bir fazdan kaçınım yatkınlığı ilkesine dayalı Fugasite Modeli'nde veri olarak kullanılıp, PCB'lerin yüzde kaçının suda, toprakta, havada, canlıda ve sedimentte toplandığı ve bu kompartmanlardaki konsantrasyonları nispi olarak hesaplanmıştır.

Sonuç olarak, Fugasite Modeli'nin varsayımları dahilinde, Poliklorlu Bifeniller'in en fazla canlıda toplandığı ve klor sayısı arttıkça canlıdaki nispi konsantrasyonun da arttığı görülmüştür.

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$a_1 \ldots a_n$	Coefficients of the characteristic equation
d_{ij}	Distance from atom i to j
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	Number of hydrogens
m_i	mole in each phase
m,n,p,..z	Valencies of vertices joined by edges
w	Wiener number
w_{ij}	weighted distance between atom i and j.
w_{ik}	All paths of length greater than zero
w_{oj}	All paths of length greater than zero
$x_1, x_2 .. x_n$	Characteristic roots of polynomials
A	Adjacency Matrix
ACM	Atom Connectivity Matrix
ACMCP	Atom Connectivity Matrix Characteristic Polynomial
C_i	Equilibrium concentration of chemical in each phase
CRI	Characteristic Root Index
D	Distance Matrix
E	Unit Matrix
HCB	Hexachloro Biphenyl and Heptachloro Biphenyl
HLC	Henry's law constant
K_{oc}	Soil sorption coefficient
K_{ow}	Octanol-water partition coefficient
K_{ps}	Soil-water partition coefficient

K_{psd}	Sediment-water partition coefficient
K_{pss}	Suspended solids-water partition coefficient
K_B	Bioconcentration Factor
K_D	Sorption coefficient
M	Total mass
Mol.ID	Molecular identification number
MHS-ACMCP	Modified Hydrogen-Suppressed - Atom Connectivity Matrix Characteristic Polynomial
P_i'	Equilibrium distribution for each compartment
P_L	Liquid vapour pressure
P(x)	Representation of the characteristic equation
PCB	Polychlorinated Biphenyl
QSAR	Quantitative-Structure Activity Relationships
QSPR	Quantitative-Structure Property Relationships
S_S	Solid Solubility
S_L	Subcooled Liquid Solubility
T	System temperature
T_1 and T_2	Characteristic Polynomial of Tree (1) and Tree (2)
T_M	Melting point
$T_r[a_{ij}]$	Trace of matrix
TCB	Trichloro Biphenyl and Tetrachloro Biphenyl
TSA	Total Surface Area
V_i	Volume of each compartment
V_A	Volume of air
V_B	Volume of biota
V_S	Volume of soil
V_{SD}	Volume of sediment
V_{SS}	Volume of suspended solids
V_W	Volume of water
WM	Weighted matrix
Z	Hosoya index
Z_i	Fugacity capacity constant of each compartment
Z_A	Fugacity capacity constant of a chemical for air
Z_B	Fugacity capacity constant of a chemical for biota
Z_S	Fugacity capacity constant of a chemical for soil

Z_{SD}	Fugacity capacity constant of a chemical for sediment
Z_{SS}	Fugacity capacity constant of a chemical for suspended solids
Z_W	Fugacity capacity constant of a chemical for water
Z^v	Number of valence electrons
%OC	Percent of organic carbon content
δ	Number of non-hydrogen bonded neighbours irrespective of multiplicity of bonding
δ_i	Count of nonhydrogen sigma-bond electrons contributed by atom i
δ^v	Count of all valence electrons (not bonding to hydrogen)
$\delta_i^{v_i}$	Count of all valence electrons (not bonding to hydrogen) including sigma electrons enumarated by δ_i
n_i	Number of lone pair electrons
$^1\chi$	First Order Molecular Connectivity Index or Randic Branching Index
$^2\chi$	Second Order Molecular Connectivity Index
ρ_S	Sorbent density
ρ_s	Density of soil
ρ_B	Density of biota
ρ_{ss}	Density of suspended solids
ρ_{sd}	Density of sediment
ρ_w	Density of water
σ	Number of bonding sigma electrons

I. INTRODUCTION

There is growing interest in the development of Quantitative Structure-Activity Relationships (QSARs) to screen and predict the toxicity and fate of chemicals released into environment.

It is well known that increasing industrialization, production and the use of chemicals have lead to a considerable increase of pollutants in the environment. It is generally accepted that before a new chemical is released into the market and thus into the environment it should undergo some assessment of its likely environmental behaviour and effects. It is hoped that such assessment will bring prior warning of hazardous or dangerous chemicals. Therefore, it is essential to predict the environmental fate of newly introduced and already used chemicals.

The modelling of the environmental fate of organic pollutants depends strongly on their distribution and requires a knowledge of certain physical properties of the chemicals in question.

In some cases, the physical property of the chemical may be unknown or there may be considerable discrepancy in the reported experimental data. Furthermore, to measure these properties for each chemical would be very expensive and time consuming. Bioconcentration tests, for example, have been estimated to cost $6000-$10000 for each chemical, and acute toxicity tests cost $2000-$3000 for each test[2]. Thus accurate estimates and/or predictions of environmental distribution coefficients are essential for any reliable ecological model that describes the environmental fate and assesses the environmental hazard of organic pollutants.

The estimation of environmentally important properties of chemicals started to draw attention in the early and mid 1970s. A universally accepted procedure for assessing the environmental fate (risks) of chemicals is not presently available. However, much effort is being directed towards developing conceptual models which simulate the behaviour of chemicals in the environment and thereby, allow assessments to a variety of chemical classes (including those that are structurally complex and contain two or more interacting functional groups). The methods must be easy to use and require a minimum of input data (the minimum being the molecular structure).

Most of the estimated methods used today for environmentally important properties of organic chemicals are based upon one of the following:

1) Theoretical equations, containing parameters that are experimentally or empirically derived. (e.g., via fragment constant)

2) Group or atomic fragment constants, sometimes structural factors, derived by regression analysis of data sets.

3) Correlations (usually in the form of linear regression equations) between two or three properties.

4) Rules for the calculation of topological indexes and the subsequent use of a correlation equation between the index and the property of interest.

Translation of molecular structure into unique characteristic structural descriptors expressed as numerical indices is used in QSAR. Potential regulation has prompted extensive work on Structure-Activity Relationships and on environmental models. Pharmaceutical and medicinal chemistry literature clearly indicates the acceptance and success of QSAR techniques in these areas. QSAR studies can be applied both to ecotoxicology of chemical compounds released into the environment and to the estimation of physicochemical properties. Interest in these methods for QSARs has developed for the following reasons:

1) Any topological index for a chemical can be calculated accurately. This accuracy allows quantitative description of the differences between two or more chemicals, and this quantification allows the development of QSARs.

2) Often, for new chemical products, only the molecular structure of the compounds composing the product are known. Topological indices require information only about the molecular structure of new compounds.

3) QSARs, using molecular structure, require no assumptions other than that, if structure is known, behaviour can be predicted.

One of the main factors that accelerated the growth in QSAR studies is the tremendous concurrent growth in computing power in terms of speed, memory, efficient algorithms for statistical analysis, interactive graphical capabilities and accuracy. New methods and techniques have begun to appear in QSAR studies using computer. Pattern recognition and cluster analysis are some of the new techniques that complement more conventional statistical approaches.

The object of this study was to derive predictive equations for physicochemical properties such as solubility, vapour pressure, octanol-water partition coefficient of PCBs, with molecular descriptors which are fundamental in nature, could be derived or calculated purely from structural information, would encode information relating to physicochemical properties and are consistent and calculable for the whole PCBs without any experimental inputs.

In making a topology based chemical prediction the first step is to apply some index to a relatively small number of well-known molecules. In general the value of the index, will differ from molecule to molecule. The next step is to construct a plot in which one axis represents the index value of the molecules and the other axis represents some chemical property, such as the molecule's boiling point. Each molecule will be represented by one point in the plot. If there is some line that fits the points well, that line can serve as the basis for

predictions because it establishes a relation between the index and the chemical property. It gives an indication of what boiling point, for example, to expect for a molecule that has a given index value. In this way the properties of well known molecules serve as a tool for predicting the properties of molecules that do not yet exist or are already present. The key to the method lies in finding the index that correlates best with the chemical or physicochemical property being studied.

Knowledge of physicochemical parameters such as the octanol-water partition coefficient, aqueous solubility, vapour pressure and Henry's constant is critically important in modelling the fate of environmental contaminants. In order to estimate the physicochemical properties of a PCB, molecular structure based on topological characteristic of molecule was characterized mathematically and these mathematically determined parameters of the molecule were correlated with tne molecule's experimentally measured properties. The derived one-variable linear regression equations were used to predict the physicochemical properties of 58 PCB congeners.

It is well known that, molecular topology determines a large number of molecular properties. The estimation of aqueous solubility was probably the first application, and it remains the subject of many QSAR studies. Hansch and co-workers[1] studied the solubility of 156 aliphatics and aromatics and derived a model using log p. In spite of the diversity among the chemicals considered, the quality of the model was found to be very good (n=156, r=0.935). Nirmalakhandan and Speece[1] obtained a strong correlation with molecular connectivity

(n=315, r=0.973). The octanol-water partition, log p, is another property that has been modelled with other descriptors. Murray[1] derived a linear one-variable model for log p using the simple first order connectivity index, $^{1}\chi$. His data set included aliphatic and aromatic esters, acids, and alcohols but excluded hydrocarbons (n=138, r=0.986).

Many other physicochemical properties have been modelled using QSAR methods for smaller data sets. Molecular connectivity has been used successfully to predict boiling points, density, heat of formation ,chromatographic retention indices[1,2,3], water solubility, octanol-water partition coefficient, molar refractivity[2], and molecular volume[2]. A data set containing all the reported soil sorption coefficients of PAHs and chlorinated HCs was recently studied by Sabljic[4,5]. He found a linear correlation with the simple first-order connectivity index, $^{1}\chi$ (n=72, r=0.976).

The success of QSAR methods and their ability to predict ecological and physicochemical properties has prompted their use in total modelling of ecosystems. In this study, the predicted physicochemical properties were used to compute the compartmentalization of PCB between air, water, soil, and sediment on the basis of Mackay's Level I Fugacity Model and then they were compared with the experimental data in the same model.

As a result, the new topological index called Characteristic Root (CR) index expressed numerically carry the topological information for a given chemical structure. So, one can easily predict the equilibrium partitioning, amount (mole)

and concentrations (ppm) of all PCB congeners in various compartments of the environment such as air, water, soil, sediment, biota, and suspended solids by using the CR index only.

II. PCBs IN THE ENVIRONMENT

Many of the chlorobenzenes and polychlorinated biphenyls are classified by the Environmental Protection Agency as hazardous waste, priority toxic pollutants, and carcinogens. PCBs were the most discussed organic pollutants initially. Although they may no longer have that distinction, they are still a serious environmental problem.

Polychlorinated biphenyls (PCBs) are mixtures obtained by fractional distillation of the products of the catalytic chlorination of biphenyl. A PCB is any one of 209 compounds of the general formula $C_{12}H_xCl_y$, where x = 0-9 and y = 10-x. 10 positions are available for chlorine atoms (labelled 2-6 and 2′-6′ in Fig.2.1.). Different structural arrangements make possible 209 compounds ranging from the three monochloro biphenyls to decachloro biphenyl.

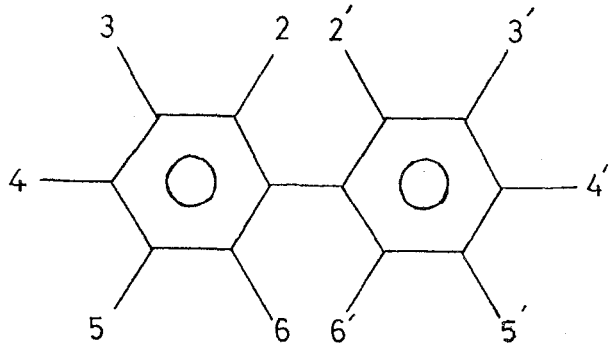


Figure 2.1. Labelling of Chlorine Atoms in the structure of PCB.

Since the early 1930s, PCBs have been used as components of dielectric fluids in transformers and capacitors, flame-resistant plasticizers, and hydraulic fluids. Later, PCBs were incorporated into paints, inks, dust control agents, carbonless paper, and pesticides. During the 1970s, national and international regulations further restricted their use. In 1976, the U.S. Congress banned the manufacture, processing, distribution and use of PCBs except in totally enclosed systems (electrical systems, capacitors, and electromagnets)(82).

The name Aroclor is frequently used interchangeably with "PCB". In fact, not all PCBs are Aroclors, but most Aroclors are mixtures of PCBs. Aroclors had been introduced into the environment in forms available for transport, transformation, or accumulation.

PCBs are still being used in 2.8 million capacitors and some 150000 transformers. Some of these fail each year and release additional quantities of PCBs into the environment.

There is also evident that certain chlorinated biphenyls can be produced in nature by the bacterial metabolism of other contaminants(87).

The characteristic properties of PCBs are hydrophobicity or lipophilicity (i.e., large octanol-water partition coefficient and low aqueous solubility), relatively low vapour pressure, and extreme resistance to chemical reaction. These properties result in persistence in the environment, a tendency to accumulate in biota and sediments and the ability to be transported through the atmosphere to regions remote from source discharges.

The presence of such a large number of congeners renders chemical analysis and reporting very difficult. A common practice has been to report environmental concentration in terms of an Aroclor grade equivalent, but this practice is imprecise because the environmental distribution of congeners differs from the commercial grade distribution. It is likely that there is differential transport, reaction and accumulation between congeners. Elucidation of the environmental transport and transformations of a mixture requires that the mixture be assigned properties such as a unique solubility or vapour pressure. Such an assignment is fundamentally erroneous because a mixture does not have unique phase equilibrium physical chemical properties. The reported measured solubilities or vapour pressures can only be regarded as some average of the properties of the individual PCB congeners.

It has became increasingly accepted that the only rigourous method of addressing the problem of calculating the environmental fate of PCBs is to obtain properties for all the congeners and treat each congener separately. Unfortunately, relatively few congeners have been synthesized in sufficient quantities for property determinations to be possible. Further, these determinations are experimental demanding and many erroneous data exist. There is now considerable interest in evaluating the potential environmental behaviour of the PCB's, and other compounds, by utilization of their physicochemical characteristics.

In this study, a tendency has been found for the congeners to have properties which vary systematically with the new CR index; thus the properties of one congener can be estimated from those of the others.

III. GRAPH THEORY

3.1. HISTORICAL BACKGROUND

Graph Theory is a subdiscipline of mathematics that is closely related to both topology and combinatorics. The origins of Graph Theory date back over 200 years. It was independently discovered on several occasions by three names- Euler, Kirchoff and Cayley. Euler[6] (1707-1783) is generally considered to be the father of graph theory. He published the first known paper on graph theory, in which he resolved the Königsberg bridge problem.

Kirschoff[7] discovered graphs while solving problems involving the calculations of currents in electrical networks. He showed that the solution could be accomplished efficiently by using the "spanning trees" of the graph represented by the given network.

Organic chemistry became the third breeding ground for graph theory. The best known early organic chemists, who founded the structure theory, were Couper, Butlerov, and Kekulé[7]. They found it convenient to represent a covalent bond between two atoms as a line joining two points; thus every structural

formula is a graph. Cayley's works, leading up to his enumeration of organic isomers, are also recognized as independent discoveries of graph theory.

Graph theory was not only a new field of mathematics, it also found applications in other disciplines. In addition to physics and chemistry, it has been applied to anthropology, architecture, civil engineering, communications, computer science, economics, electrical engineering, genetics, geography, industrial management, linguistics, operations research, political science, psychology, and sociology.

3.2. CHEMICAL APPLICATIONS OF GRAPH THEORY

The use of graphs to depict molecules was the first application of graph theory to chemistry. Within chemistry, graph theory has been applied to problems from a wide range of research areas: synthetic chemistry, polymer chemistry, quantum chemistry, petroleum chemistry, chemical kinetics, statistical mechanics, phase equilibria, spectroscopic analysis, Hückel theory, and chemical information storage and retrieval.

In recent years a large number of fairly extensive nomenclature systems based on graph theory, have been devised both for the representation and for the computer searching of structures.

Molecular structures in graph theory have been represented in different ways such as codes, matrices or polynomials, depending upon the nature of the problem. Read[8], described in detail a method whereby a unique designation (or "code") of any chemical compound can be derived from its structural formula,

in 1982. Bawden[9] reviewed applications of computerized structure-handling techniques to studies of the relationships between molecular properties and chemical structure.

Methods based on the representation of structures by matrices and polynomials have also proved to their value in computerizing chemical information. In a system used by Spialter[10], the graph of a molecule was represented in the form of a matrix, which was called Atom Connectivity Matrix. This is going to be illustrated in more detail in the coming sections.

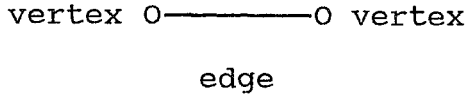
The most common method of transposing the graph of a molecule into matrix notation is via the topological or structural matrix, better known in graph theoretical language as the adjacency matrix. It was first demonstrated in 1956 by Gunthard and Primas[11] that the adjacency matrix of a molecule may be used in place of the Hückel matrix of Molecular Orbital Theory. In the Hückel Molecular Orbital Theory, each atom in an aromatic or conjugated unsaturated molecule is assumed to be connected to other atoms through the network of the overlapping π-electron domain. The spectrum of eigenvalues obtained from the graphical approach were found to be closely related to the energy levels obtained from the Hückel matrix. So the terms eigenvalue and energy level are used interchangeably in this context. The adjacency matrix was featured prominently in a study by Kettle and Tomlinson[11] of the electronic structure of boron hydrides. England and Ruedenberg[11] utilized the adjacency matrix in a calculation of the energy of localized π-orbitals for a number of aromatic hydrocarbons.

The characteristic polynomial is also used in the derivation of indices in graph theory. This polynomial is obtained by evaluating the matrix as a determinant through the usual mathematical techniques. The reduction of a graph or topological matrix to a topological index has been developed recently. Most approaches to the development of topological indices involve methods for counting selected topological features. Graph characteristics considered include examples such as the number of pairs of atoms separated by tree bonds. In QSAR studies, the most widely used index is the "valence molecular connectivity index" which has been proposed by "Kier and Hall"[3] in the derivation of physical properties of molecules. The approach quantizies the molecular structure encoding information about size, branching, cyclization, unsaturation, and heteroatom content. The structural information encoded within a topological representation of a molecule provide the basis for relating molecular structure to additive (e.g., molar volume) and constitutive properties (e.g., water solubility)[12].

Before going into the details of the valence connectivity and other indices, in order to ensure an understanding of the terms used in graph theory and their interrelations within graph theoretical concepts, some basic ideas and some definitions from graph theory will be introduced in the following section.

3.3. FUNDAMENTALS OF GRAPH THEORY

Mathematically a graph is a pair of sets, (1) a set of elements, and (2) a set of pairs of these elements. It is much easier, however, to conceive of a graph in terms of its pictorial representation, that is (1) a set of points, and (2) a set of lines that join some or all pairs of points. In other words a graph is a set of points called vertices ,which are connected by lines called edges.



The nomenclature of graph theory has not been standardized; points are also referred to as nodes and junctions, and lines as arcs and branches. No edge begins and ends at the same vertex.

Many of the terms and concepts in graph theory have their counterparts in the vocabulary of the chemist. A graph; in more general terms, is a mathematical structure which may be used to depict the topology of any given system. So, it is a topological concept rather than a geometrical concept, and hence metric lengths, angles, and three-dimensional spatial configurations have no meaning.

The word "graph", should not be confused with the Cartesian graph (e.g., y versus x) commonly used in science and mathematics to present the relationship between two or more variables visually.

Two points joined by a line are adjacent points, while two lines having a point in common are adjacent lines. The degree of a point is the number of lines joined to it. A walk is an alternating sequence of points and lines that begins with a point and ends with a point. A path is a walk in which no point occurs more than once. A connected graph has every pair of points joined by a path. A cyclic graph must include at least one walk of three or more points that begins and ends with the same point and contains no point occurs more than once (except for the first and last). A tree is a connected acyclic graph. The distance between two points is the number of lines in the shortest path joining the two points. Fig.3.1. includes a number of different graphs, and Fig.3.2. exemplifies a number of different graph theory concepts.

Graphs used in chemistry generally belong to one of two broad categories: (1) structural graphs, also referred to as chemical graphs, or constitutional graphs, and (2) reaction graphs. As the name suggests, a structural graph corresponds to a specific chemical structure, while a reaction graph corresponds to a set of chemical reactions. Reaction graphs have found their principal application in chemical kinetics and computer-assisted organic synthesis[6]. Table 3.1. provides a list of graph theory concepts and the corresponding terms used in chemistry for each of these two types of graphs.

Chemists employ various types of names and formulas when they wish to communicate information about chemicals and their structures. For the most part, however, names and formulas have no direct, immediate, or explicit mathematical meaning.

Graph theory, on the other hand, provides many different methods of characterizing structures numerically. Fig.3.3. gives IUPAC name of a chemical, its structural formula, and the chemical graph that corresponds to its hydrogen-depleted structure. A common feature of the various topological methods is the use of the hydrogen-suppressed graph, defined as the graph of the molecule excluding all hydrogen atoms. In chemical graphs the hydrogen atoms are often omitted, because they normally do not play a major role in determination of the structure of a molecule.

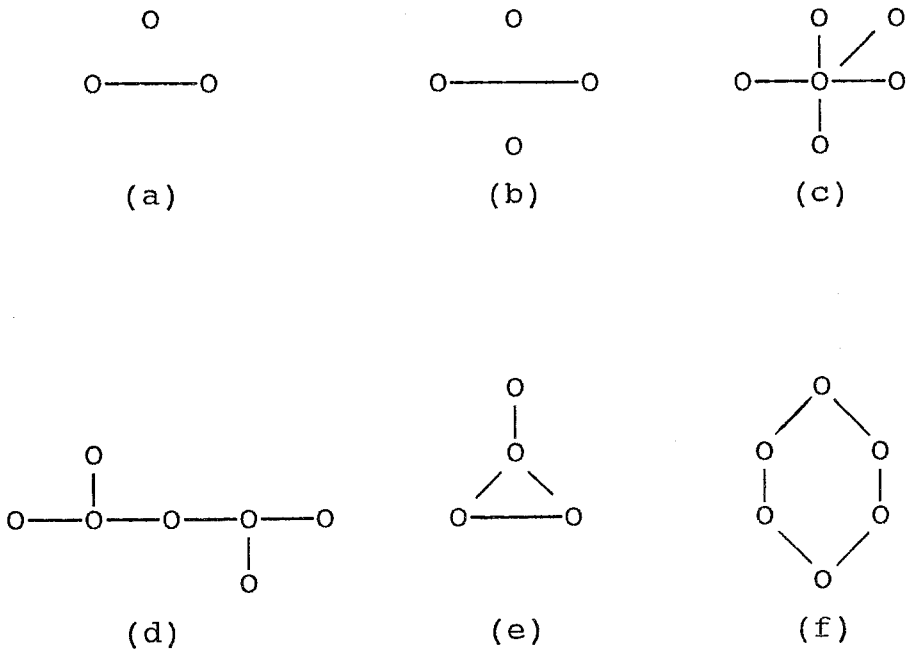


Figure 3.1. Graphs a and b are disconnected, but all of the other graphs are connected. Graphs c and d are trees. Graphs e and f are cyclic.

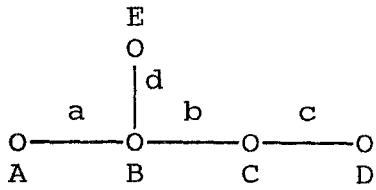
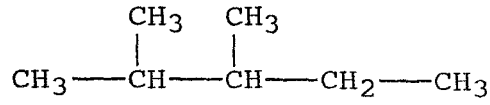


Figure 3.2. Pairs of adjacent points are AB, BC, BE, and CD. Pairs of adjacent lines are ab, ad, bd, and bc. Points A, D, and E are of degree 1, point C of degree 2, and point B of degree 3. One example of a walk is CbBdEdBaA. A path of length 2 is EdBbC. Points D and E are separated by a distance of 3.

Table 3.1. Corresponding Concepts in Graph Theory and Chemistry

Graph Theory	Chemistry	
Graph	Structural Graph	Reaction Graph
point	atom	chemical species
line	chemical bond	chemical reaction
path	chemical substructure	reaction sequence
degree	atom valency	
cyclic graph	ring compounds	
tree	acyclic structure	



2,3-Dimethylpentane

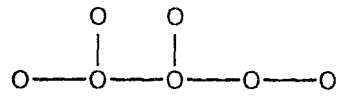


Figure 3.3. 2,3-Dimethylpentane represented as structural formula, IUPAC name and structural graph.

3.4. TOPOLOGICAL MATRICES IN GRAPH THEORY

Sylvester[7] indicated that a chemical graph could readily be converted into matrix format. For many purposes the topological matrix has proved even more useful than the chemical graph, as it provides a representation of the topology of a species in terms of numbers rather than by a diagram.

The adjacency matrix is defined such that each element a_{ij} equals 1, if and only if atoms i and j are adjacent (i.e., bonded to each other) while all other a_{ij}'s equal zero. The matrix is symmetrical and has zeros along the main diagonal. The actual form of the adjacency matrix for a given graph depends on the particular numbering of the atoms (vertices). The distance matrix is defined such that each element d_{ij} equals the length of the shortest path (i.e., the fewest number of bonds) joining atoms i and j (Fig.3.4.).

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$D = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 2 & 3 \\ 1 & 0 & 1 & 2 & 3 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 3 & 2 \\ 4 & 3 & 2 & 1 & 0 & 4 & 3 \\ 2 & 1 & 2 & 3 & 4 & 0 & 3 \\ 3 & 2 & 1 & 2 & 3 & 3 & 0 \end{bmatrix}$$

Figure 3.4. 2,3-Dimethylpentane Represented as Adjacency Matrix, and Distance Matrix.

A different but related matrix which also encodes the structure of the molecule put forward by Spialter[10] is the Atom Connectivity Matrix (ACM). The ACM is a matrix array composed of mathematical elements a_{ij}, where i and j are integers defining the rows and columns respectively, at whose intersection a_{ij} is situated. In the diagonal elements, where i = j, are placed symbols for the atoms, radicals, electrons, charges, or other constituent groups making up the molecular formula. Order of assignment is unimportant. Every atom; is defined by its

connectivities with all other atoms, and the final array, properly detailed, can represent only one skeletal linkage or bonded arrangement of its components. The matrix differs from the adjacency matrix in two respects:

-On the main diagonal the chemical elements are displayed instead of zeros. An atom is not considered as being bonded to itself.

-Off the main diagonal, bond parameters describing the bonds, such as bond orders 1,2,3 (or fractional ones) are displayed. Illustrative examples of ACM's for given molecular structures are shown in Fig.3.5.

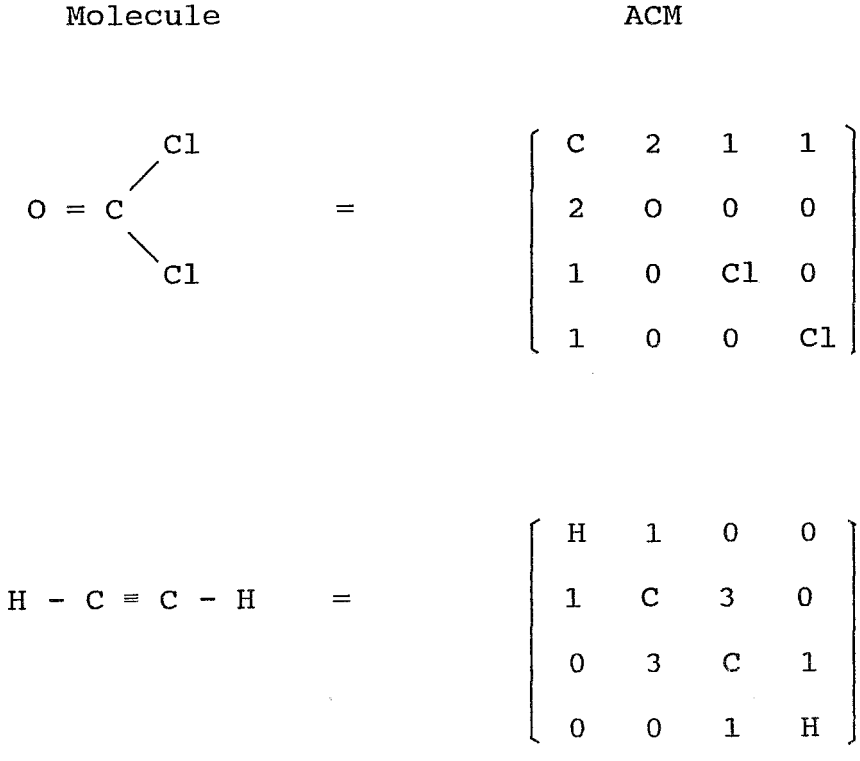


Fig.3.5. Atom Connectivity Matrix of Phosgene and Acetylene.

For large molecules ACM may appear as a formidable array. In order to save in the size of ACM, hydrogens are omitted from ACM with no significant loss in general. The saving in time and size is evident from the following examples of "hydrogen-suppressed" ACM's (Fig.3.6.).

Spialter[13] has investigated ACM for free radicals, ions, covalent alkyl halides, ionic salts, clatharates, transition states and macromolecules.

Name	Structure (Hydrogen-Suppressed)	ACM
Ethanol	C - C - O	$\begin{vmatrix} C & 1 & 0 \\ 1 & C & 1 \\ 0 & 1 & O \end{vmatrix}$
Ketene	C = C = O	$\begin{vmatrix} C & 2 & 0 \\ 2 & C & 2 \\ 0 & 2 & O \end{vmatrix}$
n-Propane	C - C - C	$\begin{vmatrix} C & 1 & 0 \\ 1 & C & 1 \\ 0 & 1 & C \end{vmatrix}$

Figure 3.6. Examples for the Hydrogen-Suppressed ACM's.

Although ACM stores the characteristics of a molecule excellently, it suffers from very serious defects. Among these are the following:

a) No method has been devised for organizing a collection of matrices in some numerical sequence defined by the matrices themselves.

b) The identity of the molecule represented by the pictograph is independent of how one cares to number or name the atoms in the molecule. This is not the case with a matrix type of representation.

c) Very complex computer operations are required to search and compare matrices.

d) Another serious handicap of matrix notation is a consequence of the quantitative exactness. ACM implies only what the chemist draws, and it is assumed that the chemist means what he draws and draws what he means.

It is evident that the storage simplicity of the matrix formulation brings along certain serious limitations with respect to searching and retrieval operations. A concept to overcome these disadvantages except for the last cited difficulty above was proposed by Spialter[13]. This concept is a mathematical "relative" to the ACM and transforms ACM into the Atom Connectivity Matrix Characteristic Polynomial (ACMCP). This polynomial is obtained by evaluating the matrix as a determinant through the usual mathematical techniques. Starting from topological matrix A, the stages in the derivation of the characteristic polynomial P(x) may be represented in the following notation:

$$A \rightarrow det \mid A + xE \mid \rightarrow \sum_{i=1}^{n} k_i x^{n-i} \rightarrow P(x)$$

where E is a unit matrix of the same size as A, x is a variable, n is the number of vertices in the original graph, and k_i is the i^{th} coefficient of the characteristic polynomial.

The following example is the ACMCP of formaldehyde

$H_2C = O$ $\quad CH^2O - 2HO - 4H^2$

The same ACMCP is obtained from any of the ACMs constructed for this molecule. So, the sequence of numbering or naming the atoms is not important. Instead of hydrogen suppressed graphs, "modified hydrogen-suppressed", or "MHS-ACMCP" was used in ACMCP. Comparison of ACMCP's for Ketene molecule is shown in the following example.

Complete ACMCP

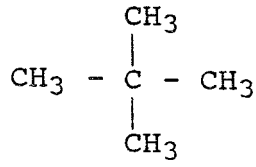
$C^2H^2O - (4CH^2 + 4H^2O + 2CHO) + 8H$

Ketene

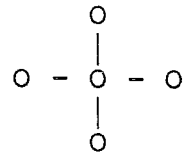
MHS-ACMCP	VC
$C^2H^2O - (4C + 4O);$	$C(1,0,2,0)$

For the hydrogen-suppressed case, the proposed appropriate polynomial includes hydrogens in the first term and an appended valency count (or VC) collection. The conjecture is that if two pictographs have identical MHS-ACMCP's they represent identical molecules at least to the extent to which information has been entered into the ACM, which may ignore stereoisomeric data.

It has been understood that characteristic polynomials contain a great deal of information about the species they represent[14]. For example, when the polynomial is set equal to zero and solved as a polynomial equation, a number of characteristic roots or eigenvalues are obtained. They can be used in the same sense as energy levels derived from a Hückel matrix. The sequence of steps required to derive the eigenvalue (characteristic root) for 2,2-Dimethylpropane from its structural graph is illustrated in Fig.3.7.



(a)



(b)

	1	2	3	4	5
1	0	1	0	0	0
2	1	0	1	1	1
3	0	1	0	0	0
4	0	1	0	0	0
5	0	1	0	0	0

(c)

$$X^5 - X^3 = 0$$

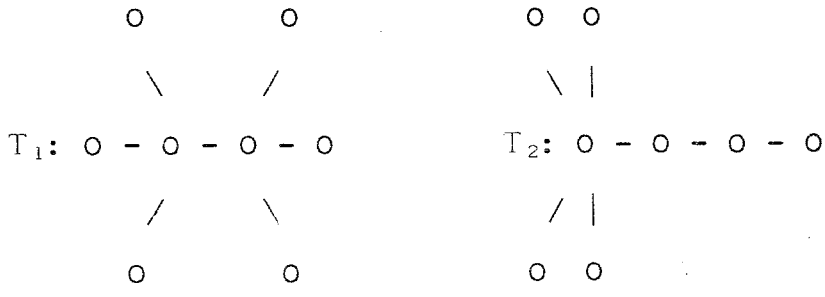
(d)

(1.0, 0, 0, 0, -1.0)

(e)

Figure 3.7. Characteristic Roots of 2,2-Dimethylpropane Derived from its Structural Formula. (a). Structural Formula, (b). Hydrogen-Suppressed Structural Graph, (c). Adjacency Matrix, (d). Characteristic polynomial, (e). Characteristic Roots or Eigenvalues.

Due to the close relationship between molecular orbital theory and graph theory, a fair amount of research on this topic[14] has been carried out to derive topology based quantities derivable from Hückel theory by the graph theoretical approach. The studies have revealed that those two matrices are equivalent and that they will therefore possess corresponding eigenvalues or energy levels. Later, it was realized that the characteristic polynomial does not uniquely determine the topology of a molecule[15]. It has been proven that nonisomorphic chemical graphs such as:



have a common characteristic polynomial which is $\emptyset(T_1)=\emptyset(T_2)=x^8-7x^6+9x^4$. So, they have the same set of characteristic roots. This has pointed out an important drawback in the use of characteristic polynomials to characterize chemical species. In this study, both the characteristic roots and characteristic polynomial derived from the chemical graph of a molecule have different values for each congener. Thus, the most important disadvantage of the characteristic polynomials/characteristic roots has been eliminated.

Another conventional methods for distinguishing the skeletons of structurally isomers have been proposed in characterization of molecular properties. These methods will be discussed in the following section.

3.5. TOPOLOGICAL INDICES AND QSAR/QSPR STUDIES

The topological method has found applications beyond the simple prediction of chemical properties. It has the potential to help in modelling and controlling corrosion, developing new anaesthetics and physcoactive drugs, in predicting the degree to which various pollutants might spread and in the environment and the harm they might do once they have spread, in estimating the carcinogenic potential of certain chemicals. Numerous attempts have been made to apply topological indices to all of these areas.

A topological index is a numerical quantity that is mathematically derived from the structural graph of a molecule. Since isomorphic graphs possess identical values for any given topological index, these indices are referred to as graph invariants. One of the earliest graph invariants or topological indices are known as vertex or carbon number, which chemists have been relying on for certain correlations for more than a century without realizing that they were using what is in fact a simple topological index. Topological indices usually reflect both molecular size and shape. Trinajstic and co-workers[6] recently reported that 39 topological indices are "presently available" in the literature.

The first reported use of a topological index in chemistry was by Wiener in his study of the boiling point of paraffin. Wiener[16] employed both a polarity number, p, which is a count of length three, and a path number, w, which is "the sum of the distances between any of two carbon atoms in the molecule, in terms of carbon-carbon bonds". Wiener number's definition has been broadened to include all nonhydrogen atoms, so that it can now be applied to nonhydrocarbons as well as hydrocarbons. The Wiener number is identically equal to one-half the sum of the elements of the distance matrix, one-half since this matrix includes the distance from atom i to atom j as well as from atom j to atom i.

$$\text{Wiener Number} = 1/2\sum d_{ij}$$

The Wiener index of a molecule provides some measure of a molecule's branching structure. After Wiener devised it, several other workers found that for certain types of hydrocarbon molecules the index correlated well with such properties as boiling point, viscosity, surface tension and refractive index.

The utility of the Wiener index is not limited to small molecules: It can be applied to polymers and crystals. The original formulation of the Wiener index when applied to an infinite polymer chain, would give an infinite value, because there would be an infinite number of paths, connecting atoms along the chain. In 1980 Bonchev and Mekenyan[17] proposed a

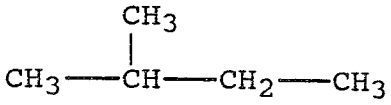
method of modifying the Wiener index so that it would yield finite values even for infinite systems, as long as the systems are composed of many identical finite units.

The Wiener number has not seen wide spread use in QSAR/ Quantitative-Structure Property (QSPR) community. It has been said, however, that its high correlation with other topological indices suggests that it deserves greater attention[6]. The Wiener index of a molecule offers primarily a measure of the molecule's volume, although it gives some indication of the molecule's shape.

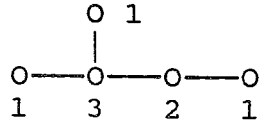
An index more sensitive to shape was introduced in 1975 by Milan Randic[18] and is known today as the Molecular Connectivity Index. It has became the most widely used index in both QSAR and QSPR studies. The Randic branching index, R, is defined as,

$$R = \sum_{\text{all bonds}} 1/(mn)^{1/2}$$

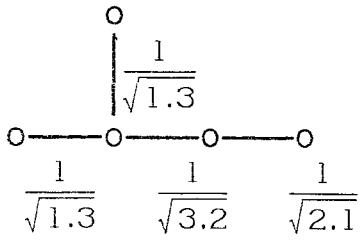
This summation includes one term for each edge in the hydrogen-suppressed structural graph. The variables m and n are the valencies of the adjacent points joined by each edge. Fig.3.8. demonstrates the sequence of steps leading from the structural formula of 2-methylbutane to its Randic branching index.



(a)



(b)



(c)

$$R = {}^{1}\chi = \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}}$$

$$= 0.5774 + 0.5774 + 0.4082 + 0.7071$$

$$= 2.2701$$

(d)

Figure 3.8. The Randic branching index (path-one molecular connectivity) of 2-methylbutane. (a) the structural formula, (b) the structural graph with the valency of each point shown, (c) the structural graph with $(1/mn)^{1/2}$ for each edge shown, and (d) the summation of $(1/mn)^{1/2}$,which yields the Randic branching index.

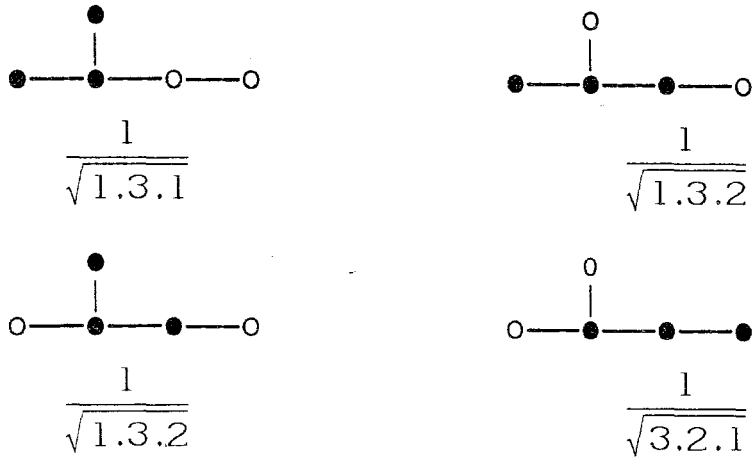
An alternative way of looking at the Randic branching index is to consider it as a summation over all paths of length one in the structural graph. The natural extension of this view is to define additional indices corresponding to paths with lengths greater than one [19], and to other subgraphs (clusters, path-clusters, and cycles) some of which may even include points of degree greater than two[6].

Hence the chemical literature now uses the term molecular connectivity to refer to as entire family of topological indices. The Randic branching index is generally referred to as the path-one molecular connectivity, $^{1}\chi$. This nomenclature is readily adaptable to the naming of the extended molecular connectivities; for example, path-two molecular connectivity or second order molecular connectivity, $^{2}\chi$, which is defined as,

$$\text{Second Order} = {}^{2}\chi = \sum^{k} 1/(mnp)^{1/2}$$

where k corresponds to all paths of length two, and m, n, and p are the valencies of the three points contained in these paths (Fig.3.9.).

The original work of Randic[18] involved only the acyclic alkanes; these, of course, represent only a very small fraction of the organic compounds of interest to chemists. Hence almost immediately the concept of molecular connectivity was altered and expanded its application to compounds containing rings[6], multiple bonds[20] and heteroatoms[21,34].



$$\text{Second Order} = {}^{2}\chi = \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{6}}$$

$$= 0.5774 + 0.4082 + 0.4082 + 0.4082$$

$$= 1.8021$$

Figure 3.9. Path-two molecular connectivity for 2-methylbutane. Each path of length two is shown in bold together with the path's contribution to ${}^{2}\chi$.

Since 1975, Kier and Hall have authored or coauthored over 35 papers in which molecular connectivities were employed in QSAR and QSPR studies.

Molecular connectivity represents perhaps the most widely used topological index (or family of indices) in QSAR and QSPR work. For example, molecular connectivity has been used in the QSAR or QSPR studies of gas chromatographic retention indices of nitrated polycyclic aromatic hydrocarbons[6], alkane solubility in water[22], rational drug design[6], halocarbon and ethers, anaesthetics[6], enzymatic reactions[23],

hallucinogenic mescaline analogs[24], bioconcentration factor of hazardous chemicals[6], chemical carcinogenicity[6], anaesthetic and toxic activity of aliphatic HCs, ethers[25], and ketones[25,26], physicochemical properties, bioconcentration and toxicity in Daphnia Pulex of PAHs[27], aqueous solubility of organic chemicals[28] and soil sorption coefficients of organic pollutants[5].

Attempting to find a topological index that would be easy to derive, unique and structurally significant, Randic[29], in 1984, proposed the molecular identification (ID) number. It is the combination of molecular connectivity and the molecular path count. More precisely, it is a weighted molecular path count in which the weights are related to molecular connectivity.

Table 3.2. gives individual and total path counts for all carbon atoms and the 2-methyl butane molecule as a whole. Fig.3.10. shows the numbering system that was assumed for this molecule. First, for mathematical completeness, paths of length zero are counted and included, these paths consist of a single point or atom. Second, except for paths of length zero, the molecular path count for any given length is not equal to the sum of the atom path counts, but rather to one half of this sum - from the fact that each of these paths has been counted twice, once from each end.

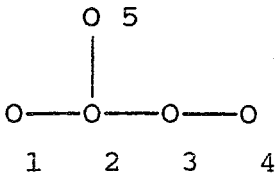
Table 3.2. Atomic and Molecular Path Counts for 2-Methylbutane.

Atom Number	Count of Path Lengths 0	1	2	3	4	Sum
1	1	1	2	1	0	5
2	1	3	1	0	0	5
3	1	2	2	0	0	5
4	1	1	1	2	0	5
5	1	1	2	1	0	5
Molecular Path Counts	5	4	4	2	0	
Molecular Path Count Total = 15						

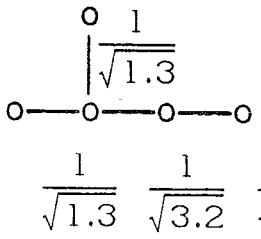
Each path of length zero is given a weight of unity. For paths of length greater than zero the weight is equal to the product of $(1/mn)^{1/2}$ terms, one term from each edge included in the path; for each of these terms m and n equal the valencies of the atoms joined by the edge. The molecular ID number is exactly analogous to the molecular path count total except that a path-weighted count is taken. Fig.3.10. shows the method used to calculate these lengths.

$$\text{Molecular ID} = \sum_{j} w_{oj} + 1/2 \sum_{ik} w_{ik}$$

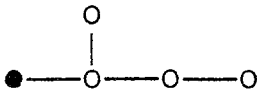
where w is the path-weight, oj corresponds to all paths of length zero and ik corresponds to all paths of length greater than zero.



(a)

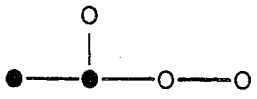


(b)



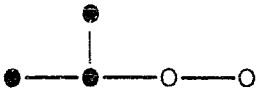
length = 0

weight = 1



length = 1

$$\text{weight} = \frac{1}{\sqrt{1.3}} = 0.5774$$

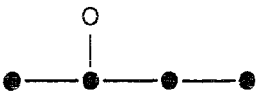


length = 2

$$\text{weight} = \frac{1}{\sqrt{1.3}} \cdot \frac{1}{\sqrt{3.1}} = 0.3333$$

length = 2

$$\text{weight} = \frac{1}{\sqrt{1.3}} \cdot \frac{1}{\sqrt{3.2}} = 0.2357$$



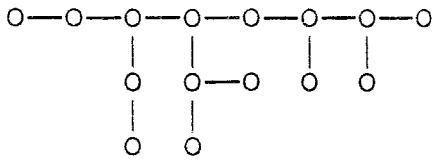
length = 3

$$\text{weight} = \frac{1}{\sqrt{1.3}} \cdot \frac{1}{\sqrt{3.2}} \cdot \frac{1}{\sqrt{2.1}} = 0.1667$$

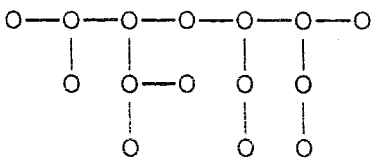
(c)

Figure 3.10. For 2-methylbutane: (a) The atom numbering system employed in Table 3.2. (b) The edge or bond weights related to the atom valencies. (c) The five paths associated with carbon atom C-1 together with their lengths and weights.

Randic[29] computed molecular ID numbers for over 400 structures (including all acyclic alkanes up to n=10 as well as a variety of monocyclics and polycyclics) and observed no degeneracy. In 1985, Trinajstic and co-workers[30] reported that their systematic examination of the 618000 alkane isomers through n=20 revealed the existence of 124 pairs and 1 trio of nonisomorphic structures with identical molecular ID numbers. For example, 2,3 - dimethyl- 6 - ethyl - 5 - isopropyloctane and 2,6 - dimethyl - 5 - ethyl - 3 - isopropyloctane both possessed the same ID number (this was true even when the ID numbers were expressed as integer expressions, precluding round-off error) (Fig.3.11.)



2,3-dimethyl-6-ethyl -5-isopropyloctane



2,6-dimethyl-5-ethyl -3-isopropyloctane

Mol.ID = $3479+3336\sqrt{2}+5844\sqrt{3}+1956\sqrt{6}/1944$ ~ 27.996462603082849972 35

Figure 3.11. Two Alkane Trees with Exactly Equal ID Indices.

Their work clearly demonstrated that the molecular ID number did not possess uniqueness. Randic[31], subsequently proposed a second molecular ID number that uses as weight the square roots of the reciprocals of the first nine prime numbers for the nine edge types commonly encountered in chemical graphs (rather than the weights based on atom valency). Trinajstic[30] also indicated that "for complicated structures the ID numbers are not easily computed. Details of this modification and other indices from the literature such as the Z index of Hosoya[32],

the Altenburg Polynomial, the Smolenski Additivity Function[3,33] and the Balaban Centric index[35] are not included in this work.

Topological indices can model an incredibly wide range of physical, chemical and biological phenomena. They can model the behaviour of gases, liquids and solids and of both inorganic and organic species. Although it has not yet been possible to tell in advance with complete certainty which index will be most suited to any particular application, various indices are already becoming known for their applicability in modelling size, shape, branching, reactivity and a large number of other characteristics. Two areas in particular where indices appear to have a bright future are in designing new drugs and in tracking the fate of various pollutants in the environment and modelling their likely effects on living organisms.

When indices are put to work, it will then be possible to make valid and useful chemical predictions of physicochemical properties of pollutants which are released into the environment. The index which is going to be used to correlate with chemical properties of pollutants must go beyond the structural fact of adjacency, which is the basis of graph theory, and should consider the valence electrons of atoms including heteroatoms participating in sigma, pi, and lone pair orbitals. In the coming sections of this work, CR index which encodes the structural differences, heteroatoms, molecular size, shape and cyclization is going to be introduced.

IV. ENVIRONMENTAL EXPOSURE ANALYSIS

4.1. MODELS FOR THE COMPARTMENTALIZATION COMPUTATIONS

This universe consists of 40000 entries amounting in an annual production of 1.8×10^{12} kg. The major part of this production (99.9 %) includes 3800 materials that are produced at rates of one million pounds/year or more[36]. Chemicals that are persistent, are subject to accumulation in biota, and those that move through the environment by unexpected pathways are of particular concern. It is necessary to make an assessment of what exposure can be expected from the introduction of a chemical into an ecosystem.

The use of compartmental analysis may provide substantial information for this type of environmental exposure prediction. With a minimum set of chemical and physical properties, consisting of vapour pressure, water solubility, and molecular weight of the chemical, a maximum environmental exposure may be predicted which takes into account the input of the chemical and its circulation within the air, soil, water and biota compartments of a simple ecosystem.

The basic process in any hazard evaluation involving the environmental effects of chemicals is to make predictions of the expected environmental concentration (EEC) and to match this with the experimentally determined no-effect level for appropriate environmental organisms. For the compartmentalization computations the following models are suggested.

Author	Basic properties	Model
Klopffer et al[37] (1979)	Molecular Mass, Water Solubility, Vapour Pressure	presumes equilibria between media
Mackay[38] (1979)	Molecular Mass, Water Solubility, Adsorption, Vapour Pressure	fugacity capacities are used to explain various compartment relationships
Neely[39] (1980)	Molecular Mass, Water Solubility, Vapour Pressure	use laboratory and monitoring data in a pond environment
Wood[37] (1980)		is independent of the compartment volume

Wood's and Mackay's models are both based on the concept of fugacity. The Klopffer[37], Mackay[38] and Wood[37] 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.

4.1.1. COMPUTATION OF ENVIRONMENTAL COMPARTMENTALIZATION ACCORDING TO NEELY

The following three equations have been proposed by Neely (1980) to predict the environmental partitioning of a chemical between the media,

- air,
- water,
- sediment/soil

% of chemical in air = - 0.247 (1/HLC) + 7.9 logS + 100.6

% of chemical in water = 0.054 (1/HLC) + 1.32

% of chemical in soil = 0.194 (1/HLC) -7.65 logS - 1.93

where

$$\text{HLC [mmHg m}^3\text{/mol]} = \frac{\text{Vapour Pressure} \times \text{Molar Mass}}{\text{Water Solubility}}$$

$$\text{S [mmol/litre]} = \frac{\text{Water Solubility}}{\text{Molar Mass}}$$

Obviously the equations use only the three physicochemical properties

- Molar mass [g/mol]
- Vapour Pressure [mm Hg]
- Water Solubility [ppm]

The computed distributions can be normalized by the following scheme.

$$N_A = \frac{\%\text{Compound Air}}{\sum \%\text{Compound (Air, Water, Sediment/Soil)}}$$

$$N_W = \frac{\%\text{Compound Water}}{\sum \%\text{Compound (Air, Water, Sediment/Soil)}}$$

$$N_S = \frac{\%\text{Compound Sediment/Soil}}{\sum \%\text{Compound(Air, Water, Sediment/Soil)}}$$

Normally the N-values have ranged between 0 and 1, but though the regression equations are constructed in such a way that the total percentage is always 100%, the value of the mass percentage in a compartment can take on any value, either positive or negative. This always happens when the relationship between the water solubility and the vapour pressure of the chemical under consideration does not fit the range used by Neely. If negative values are obtained in a compartment, the result is taken as zero and results far in excess of 100 % are taken as 100 %. If two compartments have values greater than 100 %, it is assumed that the chemical has split between the two compartments.

4.1.2. COMPUTATION ACCORDING TO MACKAY

The Mackay approach utilizes the concept of fugacity[38,40,41], which can be defined as the tendency for a substance to escape from a phase and assumes that:

1) Equilibrium conditions exist among a set of environmental

compartments.

2) The environment is a closed system consisting of the air (A), water (W), sediment (SD), soil (S), and aquatic biota (B) compartments.

3) No degradation process occurs during the distribution.

This model also accepted by OECD, consists of 1 km square with 20 km high atmosphere; 30 % of the area is covered by soil whose depth is 3 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 0.5 ppm of biota.

The organic carbon contents are 2 % for soil and 4% for sediment and suspended solids. A temperature of 25° C is assumed and the total amount of solute is arbitrarily taken as 100 moles. It results in the general equation:

$$P_i = \frac{Z_i \times V_i}{\sum_i V_i \times Z_i} \qquad (i = A, W, S)$$

with the fugacity capacities:

$$Z_{Air} = \frac{1}{RT}$$

$$Z_{Water} = \frac{1}{HLC}$$

$$Z_{Soil/Sediment} = \frac{K_D \rho_S}{HLC}$$

$$Z_{Biota} = \frac{K_{ow} B}{HLC}$$

where

R (J/mol°K) = Universal Gas Constant

T (°K) = Absolute Temperature

HLC (Pa m^3/mol) = Henry's Law Constant

$K_D \frac{m^3 water}{10^6 sorbent}$ = Sorption Coefficient

$$= \frac{K_{oc} \times \% \text{ organic carbon content}}{100}$$

ρ_S (g/cm^3) = Sorbent Density

B = Mass Fraction of Biota Times Total Biota or Lipid Part

K_{oc} = Soil Sorption Coefficient

K_{ow} = Partition Coefficient

and the volumes V_A, V_W, V_S of the environmental compartments air, water and soil/sediment which are listed in Table 4.1.

Table 4.1. Properties of the Unit World.

Compartment	Volume (m^3)	Media Densities (kg/m^3)
Air	6×10^9	1.19
Soil	4.5×10^4	1500
Water	7×10^6	1000
Biota	7	1000
Suspended Solids	35	1500
Sediment	2.1×10^4	1500

Obviously the physicochemical data needed are,

- Molar Mass
- Water Solubility
- Vapour Pressure
- Soil Sorption Constant
- Partition Coefficient

The total mass distributions provide only one component of the information needed for a meaningful hazard assessment. In addition, it is important to know the distribution of the chemical in terms of concentrations.

However, using the basic equations of Mackay's fugacity approach;

$$C_i = Z_i f_i$$

where

C_i and f_i are the concentration and fugacity respectively of the chemical under consideration in the compartment i. Z_i is the fugacity capacity constant at equilibrium.

Although this model is quite hypothetical due to its ignorance of transformation, and of biological and chemical degradation processes, it represents a picture of ultimate environmental distribution in terms of both relative concentrations and relative masses providing comparative exposure information.

It is generally accepted that such models should be validated by comparison with real environmental data. However, since models of this type do not describe any particular real environment, results can only be validated general comparison of the observed environmental concentrations and of predicted values based on direct calculation by using the observed data.

In this study, experimental physicochemical property data taken from the literature were used to compute the distribution of PCBs in various compartments on the basis of Mackay's Level I Fugacity Model and the input data needed for the Model, such as water solubility, octanol-water partition coefficient and vapour pressure, were predicted by using the CR index and used to determine the compartmentalization of PCBs in the same model. Then ,the results were compared in plots of equilibrium distribution (%), mass distribution (%), and concentration (ppm) in section V.

In order to compute the environmental compartmentalization of PCBs a BASIC program was written which is suitable for personal computers (such as IBM PS/2 model 30-H21).

V. ESTIMATION OF PHYSICOCHEMICAL PROPERTIES OF PCBs USING THE CR INDEX

5.1. DERIVATION OF THE CR INDEX

Techniques for automatic handling of chemical structure representations, within computerized chemical information systems are well developed for information storage and retrieval[9]. Such techniques are being increasingly applied to studies of structure-property relationships, involving a variety of molecular properties. The simplest types of structural feature which may be used are counts of the most basic structural units present: total number of atoms, bonds, or rings, occurrence of particular atoms, multiple bonds, etc. Features of this sort are frequently used as part of a mixed descriptor. Other structural descriptors are based on "paths" of atoms and bonds through the structure.

The purposes of topological indices are

(a) to classify structure and

(b) to serve for structure-property correlations.

Several review papers on topological indices were published in the past years such as Wiener number[10], Gutman's M_1[42],

Hosoya's Z[43], Randic's Connectivity Index $^{1}\chi$[18], Balaban's Centric Index[36], etc. They all failed to be unique, although they showed different degrees of discrimination among closely related structures.

The connectivity index which is based on differentiation of bond types and uses different weight factors for different bonds, appears to be the most successful in producing structure-property correlations and regressions, particularly when suitably expanded to account for differentiation among heteroatoms. An index that is highly selective and could at the same time be successful in correlating many different properties has not been discovered yet. However, one should hardly expect that another undiscovered index may be superior to the reported indices in literature.

The task of this study was to represent each structure by a single parameter, by the derivation of the CR index. The CR index is a hybrid of valence connectivity, path counts and distance matrix. The CR index comprises valence values and path counts used in valence connectivity; more information about the significance of this approach will be given in section 5.1.1.

The starting point of the derivation of the CR index was to draw the structural graph of a molecule and write the valence degree of each vertex (atom), listed in Table 5.1. The next step was arbitrarily labelling the vertices of the graph representing the structure. The characteristic polynomial of the molecule represented by the matrix is independent of how one cares to number the atoms in the structural graph. The derivation of the CR index was easily carried out by the

construction of a topological matrix which is called the weighted matrix, (WM). The matrix, WM, is a square $p \times p$ matrix which is converted to a characteristic polynomial by using Bocher's formula[60] which states that the sum of the diagonal elements of a square matrix is equal to the sum of its characteristic value.

The topological distance w_{ij} between two vertices i and j equals to the inverse square root of the product of the valence degrees of the vertices along the path concerned. Then, by definition w_{ij} is a weighted path number which appears in matrix WM, at the intersection of row/column i/j and j/i.

$$w_{ij} = \sum_{i}^{j} (1/mnp...z)^{-1/2} \qquad (5.1)$$

where m, n, p,...z are the valence degree of each vertex along the weighted path. The number of vertex valencies that appear in the formula depends on the number of vertices along the path i and j, which joins the vertex i and j. So, the entries, w_{ij}, of the matrix were calculated by considering the smallest distance to any other vertex. For cyclic structural graphs, (for example, benzene) when there are two equal shortest paths, the clockwise direction path count is proposed. Path counts preserve some information on more distant neighbours. The main diagonal of the matrix WM contains only zeros, because there is no path bonding to the atom itself. So, entries of this sort (w_{ii}, w_{jj}) are zero. After the matrix was constructed , it was stored in a computer program which was written in TURBO PASCAL for personal computer (IBM PS/2 model 30H21). This program is given in Appendix IV. The input data of the program were the

entries, w_{ij}, of the matrix. One program stored the matrix, the other program converted the stored matrix into characteristic polynomial form. The output data comprised the coefficients of the characteristic polynomial of the matrix constructed. The computer program uses the following algebraic techniques for the conversion of the matrix to the characteristic polynomial.

The general form of the characteristic equation is

$$P(x) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + \ldots\ldots + a_{n-1} x + a_n = 0$$

The coefficients of the various powers of x can be obtained in terms of the characteristic values of matrix, A. For example, the coefficients of x^{n-1} are

$$a_1 = (x_1 + x_2 + x_3 + \ldots\ldots x_n)$$

It is found that the coefficient of x^{n-1} is equal to the negative sum of the diagonal elements of matrix, A, i.e.,

$$a_1 = -(x_1 + x_2 + \ldots\ldots + x_n)$$

$$= -(a_{11} + a_{22} + \ldots\ldots + a_{nn})$$

The sum of the diagonal elements of a matrix is given a special name and it is called the "trace" of the matrix. Hence the above relation can be written as

$$x_1 + x_2 + \ldots\ldots + x_n = \text{trace of } A$$

$$T_r[a_{ij}] = a_{11} + a_{22} + \ldots\ldots + a_{nn}$$

If the trace of A^k (A multiplied by itself k times) is given the symbol T_k, then a useful recursive formula for expressing the coefficients of the characteristic equation in terms of the various T_k can be written as

$$a_1 = -T_1$$

$$a_2 = -\frac{1}{2}(a_1 T_1 + T_2)$$

$$a_3 = -\frac{1}{3}(a_2 T_1 + a_1 T_2 + T_3)$$

.....

$$a_n = -\frac{1}{2}(a_{n-1} T_1 + a_{n-2} T_2 + \ldots + a_1 T_{n-1} + T_n)$$

and is called Bocher's[60] formula. So, it is more helpful if a computer is to be used to determine the coefficients in the characteristic equation. Thus, structural graphs of 58 PCB congeners were converted into polynomial form (Appendix II). The final step was to find the roots of the characteristic polynomial. Eureka packet program was used to compute the characteristic roots of the polynomials. This time, the coefficients of polynomials were used as input data for Eureka package.

The characteristic root (CR) index was obtained by summing up the positive characteristic roots. Preliminary studies on the new index had shown that the best correlation was obtained for each property if total positive roots were considered. For linear, acyclic, and cyclic symmetrical molecules, constructed matrices were symmetrical about the main diagonal, since each of the paths was being counted twice, once from each end. So, the total positive roots were equal to the total negative roots. On the other hand, for asymmetrical cyclic molecules, they are not equal because of the difference between entries of the upper

and lower triangle of the matrix, meaning w_{ij} was different than w_{ji}. The reason for this was counting the paths in clockwise direction in each case.

As a result of this, the calculated (CR) indices of PCBs having the same number of chlorine atoms at different positions comprised different value from each other. So each congener was characterized by a single number.

One of the purposes of this study was to determine to what degree the CR index was suitable for the prediction of properties needed for the environmental distribution model of a chemical.

5.1.1. SIGNIFICANCE OF VALENCE DEGREES OF ATOMS

In molecular connectivity theory, the most critical aspect of the relation between molecular topology and properties is the dependence on vertex valence. The connectivity index is the valence-weighted counts of connected graphs. Within the context of molecular connectivity, an atom in its valence state can be described by two cardinal numbers; δ , the number of bonded neighbours (excluding hydrogen), and δ^{v} , the number of valence electrons (excluding those bonding hydrogen).

It is apparent that δ_i is a count of the nonhydrogen sigma-bond electrons contributed by atom i. δ^{v}, is a more inclusive count of all valence electrons (not bonding to hydrogen), including those sigma electrons enumerated by δ_i. Thus the relationship is;

$$\delta_i^{v_i} = \delta_i + p_i + n_i = \sigma_i + p_i + n_i - h_i$$

where p_i is the number of p orbital electrons and n_i is the number of lone-pair electrons on atom i. The values of δ^v and δ depend on the element represented, its valence (hybrid) state and the number of bonded hydrogen atoms.

It might be anticipated that the information available from δ_i^v and δ_i, when formulated into bond descriptions and ultimately summed to a molecular value, would be of considerable utility in counting molecules according to physical and chemical property values.

Two basically different kinds of information are encoded in δ^v and δ values of atoms. First, since δ^v and δ count sigma, π, and lone pair orbitals, it is expected that the space occupied by these orbitals might be described. This orbital space defines the expanse of the atom in its valence state due to the number and kind of orbital domains of the atom.

The second type of information expected from the δ^v and δ values of a covalently bond atom is of an electronic character. The numbers of sigma, π and lone-pair electrons must govern certain electronic properties that may be closely related to δ^v and δ of the atoms. When translated into bonds and molecules, this electronic information may bear a significant relationship to certain molecular properties. The δ^v and δ values contain information about electron domains or orbitals associated with atoms. Thus a volume characteristic is encoded in the δ values. As a result, molecular connectivity contains the properties of electronegativity and volume encoded in δ_A^v for atom (A) which are considered to be contributed equally from all valence electrons or their orbitals. Thus, one electron from atom A

forming one σ bond will possess the fraction $1/\delta_A^v$ of the properties encoded in δ_A^v. Atom A brings to the bond A-B the fraction $1/\delta_A^v$ of the properties encoded by δ_A^v. Atom B brings to the same bond the fraction $1/\delta_B^v$ of the properties encoded by δ_B^v.

If the property under consideration is the electronegativity, then orbitals from A and B contributing the fractions $1/\delta_A^v$ and $1/\delta_B^v$, respectively, will become adjusted toward an equal intermediate electronegativity, which may be ascribed to the bond. This principle of electronegativity equalization was set forth by Sonderson[43], who proposed that the geometric mean of the atom electronegativities leads to the best description of the bond electronegativity.

From Sonderson[44], $[(1/\delta_A^v)(1/\delta_B^v)]^{1/2}$ is the algorithm for two bonded atoms. This algorithm is identical to the molecular connectivity description of a bond. The volume contributed by atom A to a bond A-B is the fraction $1/\delta_A^v$ of the total. The fraction $1/\delta_B^v$ is the volume contributed from atom B. The bond has a "volume" due to orbital overlap that can be approximated by $2[(1/\delta_A^v)(1/\delta_B^v)]^{1/2}$. With a constant of 2, $[(1/\delta_A^v)(1/\delta_B^v)]^{1/2}$ reflects the relative value of the bond A-B. This is the same expression describing the electronegativity of the A-B bond which was stated above.

It has been stated that hydrogen atoms are "suppressed" in the count of valence electrons and bonding neighbours to an atom. Thus:

$$\delta^v = Z^v - h$$

$$\delta = \sigma - h$$

where Z^v is the number of valence electrons, h is the number of hydrogens, and σ is the number of bonding sigma electrons. The hydrogen influence in reality is subsumed into modified δ^v and δ values reflecting the number of hydrogen atoms on the atom in question. Using the expression $\delta^v = Z^v - h$, the valence for oxygen and nitrogen in several variations of bonding can be calculated.

Ammonia and water are unique limiting case of the $Z^v - h$ expression. The nitro group nitrogen has a valence degree of 6, since it can be considered to be derived from a nitroso group by appending another connection, namely an oxygen atom bonded to the nitrogen atom. The nitrogen atom of a tetra alkylammonium ion is, by the same argument, assigned a valence degree of 6. The improvement in the correlations[3,21] with the boiling point and molar refraction for a wide range of molecules suggests the general applicability of these values.

One approach to the connectivity of halogens has been to develop empirical values of valencies. The object was to create valence degree values consistent with carbon, nitrogen, and oxygen. The empirical valence degree values are listed in Table 5.1. In the construction of the matrix, the entries were calculated the using valence degree values in Table 5.1.

Table 5.1. Valence degree values for Heteroatoms(44)

Group	Valence degree	Group	Valence degree
NH_2	3	OH	5
NH	4	O	6
N	5	C=O	6
$C \equiv N$	5	Furan O	6
C=NH	4	O=NO	6
Pyridine N	5	H_2O	4
Nitro N	6	H_3O^+	3
NH_3	2	F	- 20
NH_4^+	1	Cl	0.69
$>N<^+$	6	Br	0.254
$=NH_2^+$	3	I	0.085

Specimen Calculation

5.1.2. CONSTRUCTION OF THE MATRIX AND COMPUTATION OF THE CHARACTERISTIC POLYNOMIAL AND CHARACTERISTIC ROOTS FOR n-PROPANE.

(a) Molecular Structure

$CH_3 - CH_2 - CH_3$

n - propane

(b) Hydrogen-depleted structural graph with vertex valencies.

O - O - O

1 2 1

(c) Arbitrarily numbering of each vertex which will form the rows and columns of the matrix, WM.

O - O - O

1 2 3

(d) Computation of matrix entries, w_{ij},

$w_{11} = 0$ $w_{21} = (2.1)^{-1/2}$ $w_{31} = (1.2.1)^{-1/2}$

$w_{12} = (1.2)^{-1/2}$ $w_{22} = 0$ $w_{32} = (1.2)^{-1/2}$

$w_{13} = (1.2.1)^{-1/2}$ $w_{23} = (2.1)^{-1/2}$ $w_{33} = 0$

(e) Constructed matrix, WM, with the above entries, w_{ij},

$$WM = \begin{pmatrix} 0.0000 & 0.7071 & 0.7071 \\ 0.7071 & 0.0000 & 0.7071 \\ 0.7071 & 0.7071 & 0.0000 \end{pmatrix}$$

(f) Computation of the coefficients of the characteristic polynomial by using Bocher's formula.

$$a_1 = T_1$$

$$a_1 = -(w_{11} + w_{22} + w_{33}) = 0$$

The matrix product of WM with itself.

$$WM^2 = \begin{pmatrix} 0.9999 & 0.4999 & 0.4999 \\ 0.4999 & 0.9999 & 0.4999 \\ 0.4999 & 0.4999 & 0.9999 \end{pmatrix}$$

$$a_2 = -\frac{1}{2}(a_1 T_1 + T_2)$$

$$T_2 = (0.9999 + 0.9999 + 0.9999)$$

$$a_2 = -\frac{1}{2}(0 + T_2)$$

$$a_2 = -\frac{1}{2}(2.9999)$$

Thus

$$a_2 = -1.4999$$

Similarly, the third power of matrix, WM,

$$WM^3 = \begin{pmatrix} 0.7068 & 1.0602 & 1.0602 \\ 1.0602 & 0.7068 & 1.0602 \\ 1.0602 & 1.0602 & 0.7068 \end{pmatrix}$$

So that

$$a_3 = -\frac{1}{3}(a_2 T_1 + a_1 T_2 + T_3)$$

$$T_3 = (0.7068 + 0.7068 + 0.7068) = 2.1204$$

$$a_3 = -\frac{1}{3}(2.1204)$$

$$a_3 = -0.7068$$

Finally the characteristic polynomial for n-propane is

$$x^3 - 1.4999x - 0.7068$$

(g) Computed characteristic roots of the polynomial of n-propane using Eureka packet program.

$$x_1 = 1.4139$$

$$x_2 = -0.7105$$

$$x_3 = -0.7204$$

(h) The characteristic root (CR) index for n-propane is 1.4139. The CR index for 58 congeners were computed in the same manner and listed with the molar mass and total surface area ($A^{\circ 2}$) of PCBs in Table 5.2.

5.1.3. PHYSICAL INTERPRETATION OF THE CR INDEX

The characteristic polynomial for a chemical species contains a great deal of information about the species it represents. For example, when the polynomial is set equal to zero and solved as a polynomial equation, a number of characteristic roots, or eigenvalues, are obtained and their number is always equal to the number of atoms in the hydrogen-suppressed structural graph of a molecule. So, the size of the structural graph is encoded in the characteristic roots. Characteristic polynomials and characteristic roots give unique characterization of each congener. The CR index seems to be closely related to the number of chlorine atoms of each congener and also gives additional information according to the configuration of the chlorine atoms. So, the isomers have a somewhat different CR index from each other without rounding off the results up to four digits after the decimal point.

The CR index can be viewed as a quantitative measure of the area occupied by the projection of the non-hydrogen skeleton of a molecule. The correlation coefficients between the CR index and calculated two sets of total surface area data taken from Opperhuizen[45] and Mackay[48] are 0.974 and 0.998 respectively. The regression equations are :

$$TSA^{(45)} = 18.56\ CRI + 182.39$$

$$n = 24;\quad r^2 = 0.949;\quad r = 0.974;\quad S_{y,x} = 4.38$$

$$TSA^{(48)} = 31.86\ CRI + 116.94$$

$$n = 27;\quad r^2 = 0.997;\quad r = 0.998;\quad S_{y,x} = 1.60$$

which allow estimation to within a factor of 4.38 and 1.60

respectively. The graphical representation of these fits are given in Fig.5.1. and Fig.5.2. These results indirectly support the physical meaning of the CR index.

Among the various types of chemical structure parameters, the total surface area (TSA) of solutes is often employed for correlations with aqueous solubility[45,48,96,97], vapour pressure[85,97], octanol-water partition coefficient[65], soil sorption coefficient[5] and Henry's Law Constant[85]. It does appear to account for several structural effects, thus very good correlations with these properties have been obtained. However, it is very difficult to determine the surface area of a molecule. One needs to know van der Waals radii, appropriate bond distances and angles. Under these conditions, estimation of the properties which depend on the total surface from the CR index may be advantageous, since it requires only knowledge of molecular structure. It can be used in the correlations instead of TSA. So, correlations of each TSA dependent property (aqueous solubility, vapour pressure, octanol-water partition coefficient, soil sorption coefficient and Henry's Law Constant) with the CR index have been investigated in the following section. The relevant data used for estimation of physicochemical properties of PCBs are given in Table 5.3. which is a compilation of water solubility (mol/l), vapour pressure (mmHg), and octanol- water partition coefficient data for PCB isomers.

Table 5.2.CHARACTERISTIC ROOT (CR) INDEX AND TSA VALUES OF PCBs.

COMPOUND	CR INDEX	MOLAR MASS	TSA ($A^{\circ 2}$)
BIPHENYL	2.4084	154.2	184.43 [81] 192.30 [67] 224.10 [45] 192.50 [45,48]
2-CHLORO	2.8928	188.7	195.45 [81] 232.30 [45] 208.40 [45,48]
4-	2.9528	188.7	202.12 [81] 209.90 [65] 237.00 [45] 210.00 [45,48]
2-2'-DICHLORO	3.4059	223.1	200.80 [81] 224.30 [65,45,48] 240.50 [45]
4-4'-	3.4741	223.1	219.81 [81] 227.40 [65] 249.90 [45] 227.60 [45,48]
2-5-	3.4553	223.1	212.97 [81] 227.59 [48]
2-6-	3.4370	223.1	206.46 [81]
2-4'-	3.4322	223.1	245.20 [45] 213.14 [81] 226.00 [45,48]
3-4-	3.4277	223.1	225.40 [65] 217.73 [81]
3-3'-	3.4472	223.1	219.47 [81]

Table 5.2.Continued

COMPOUND	CR INDEX	MOLAR MASS	TSA ($A^{\circ 2}$)
2-2′-4-	3.9340	257.5	218.50 [81]
2-2′-3-	3.9469	257.5	215.69 [81]
2-2′-5-	3.9522	257.5	218.32 [81] 241.80 [65,45,48] 253.40 [45]
2-4′-5-	3.9311	257.5	230.66 [81] 258.10 [45]
2-3-3′-	3.9243	257.5	227.86 [81]
2-3-4′-	3.9640	257.5	228.03 [81]
3-4-4′-	3.8857	257.5	235.42 [81] 243.18 [48]
2-4-4′-	3.8900	257.5	230.83 [81] 258.10 [45] 234.60 [45] 243.58 [48]
2-4-5-	3.9301	257.5	228.74 [81] 241.40 [65] 255.60 [45] 242.00 [45]
2-4-6-	3.9426	257.5	224.16 [81] 243.40 [65] 252.70 [45]
2-2′-3-4-	4.4231	292.0	231.47 [81]
2-2′-3-5′-	4.4637	292.0	
2-2′-4-4′-	4.4487	292.0	236.19 [81] 266.30 [45] 259.60 [45]
2-3-4-4′-	4.3185	292.0	243.80 [81] 266.30 [45] 259.60 [45,48]
2-2′-5-5′-	4.4941	292.0	235.84 [81] 266.30 [45] 259.60 [45,48]
2-3′-4-4′-	4.4418	292.0	264.44 [81] 268.50 [45] 259.20 [45,48]
2-3′-4′-5-	4.4757	292.0	268.50 [45] 246.26 [81] 259.20 [45,48]

Table 5.2. Continued

COMPOUND	CR INDEX	MOLAR MASS	TSA ($A^{\circ 2}$)
2-2′-3-3′-	4.4149	292.0	230.58 [81] 261.30 [45] 255.60 [45,48]
2-2′-6-6′-	4.4192	292.0	217.18 [81] 246.70 [45]
3-3′-4-4′-	4.4345	292.0	270.70 [45] 251.02 [81] 267.60 [45] 258.76 [48]
2-3-5-6-	4.1870	292.0	236.24 [81]
2-4-4′-5-	4.4137	292.0	246.23 [81]
2-3-4-5-	4.3470	292.0	241.72 [81] 255.21 [48]
2-2′-5-6′-	4.4766	292.0	229.34 [81]
2-2′-4-5-	4.4613	292.0	234.10 [81]
2-3′-4-4′-5-	4.9159	326.4	262.04 [81]
2-3′-4-4′-5-	4.9159	326.4	262.04 [81]
2-3-3′-4-4′-	4.8980	326.4	259.41 [81]
2-3-4-5-6-	4.8166	326.4	250.10 [81] 271.70 [45] 269.20 [45,48]
2-2′-3-4-4′-	4.9049	326.4	249.16 [82]
2-2′-3-5′-6-	4.9561	326.4	244.23 [82]
2-2′-4-6-6′-	4.9363	326.4	234.87 [82]
2-2′-3-4-5′-	4.9391	326.4	246.43 [81] 276.70 [45] 273.20 [45,48]
2-2′-3′-4-5-	4.8907	326.4	
2-2′-4-4′-5-	4.9311	326.4	251.79 [81]
2-2′-4-5-5′-	4.9718	326.4	251.62 [81] 275.00 [65] 276.70 [45] 275.20 [48]
2-3-3′-4′-6-	4.8933	326.4	254.65 [81]

Table 5.2, Continued

COMPOUND	CR INDEX	MOLAR MASS	TSA ($A^{\circ 2}$)
22'-33'-66'-	5.3998	360.9	246.95 [81] 287.40 [65] 269.50 [45]
22'-3-44'-5-	5.3200	360.9	264.76 [81]
22'-3-4-55'-	5.4014	360.9	264.59 [81]
22'-3-4'-55'-	5.3902	360.9	266.51 [81]
22'-44'-55'-	5.3952	360.9	267.39 [81] 290.50 [65] 287.10 [45] 290.80 [45,48]
22'-4-55'-6-	5.4492	360.9	
22'-33'-44'-	5.3125	360.9	262.13 [81] 282.10 [45] 286.80 [45,48]
22'-44'-66'-	5.5348	360.9	252.56 [82] 272.50 [45] 291.50 [45,48]
22'-33'-44'-6-	5.8473	395.3	289.90 [45]
22'-33'-44'-55'-	6.3039	429.8	293.34 [81] 302.90 [45] 317.90 [45,48]
22'-33'-4-5'-66'-	6.3872	429.8	277.62 [81]
22'-33'-55'-66'-	6.3834	429.8	393.30 [45] 276.73 [81] 318.50 [65] 318.70 [45,48]

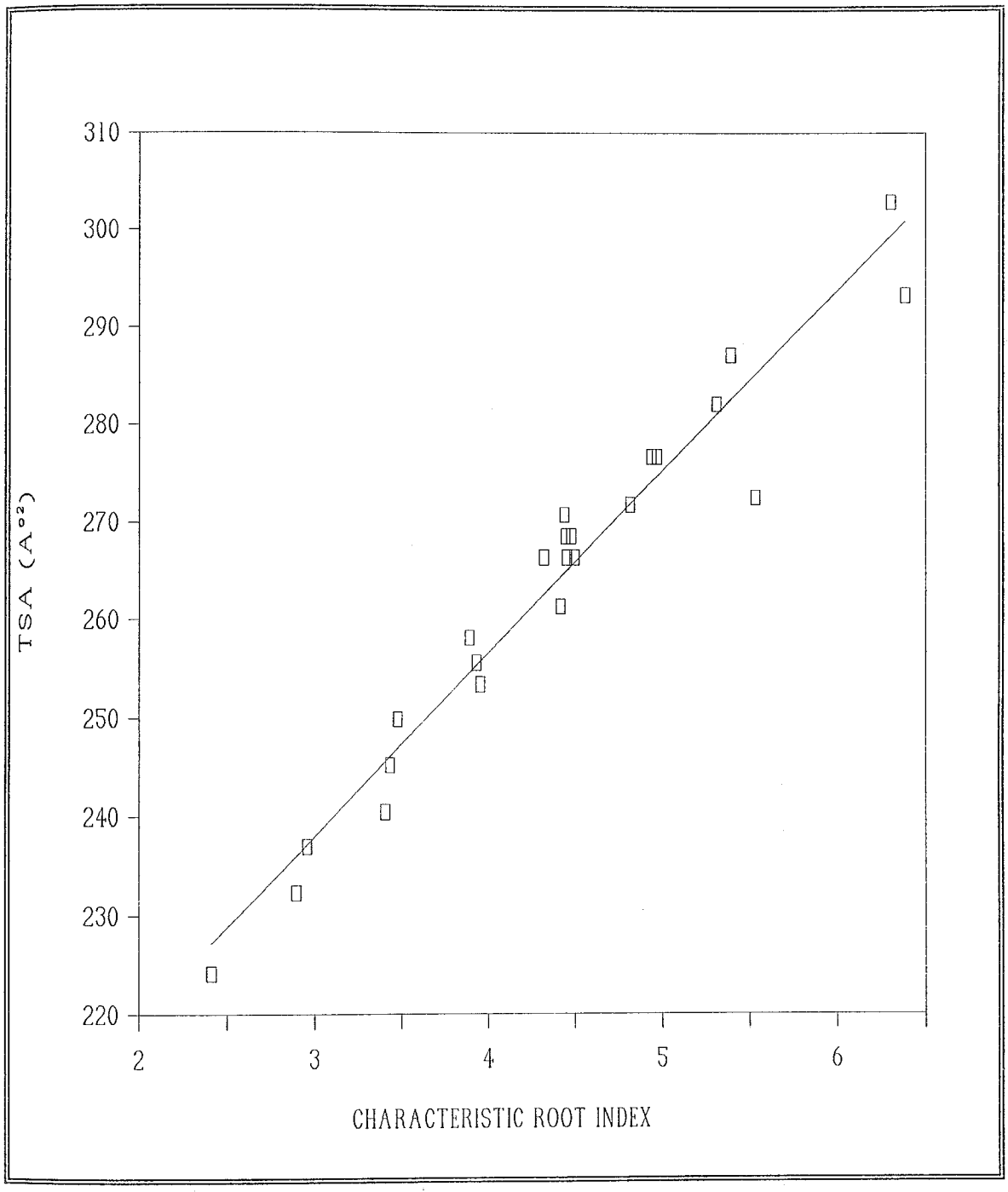


Figure 5.1. The total surface areas plotted as a function of the characteristic root indices of 24 PCBs from Table 5.2. and Ref.45.

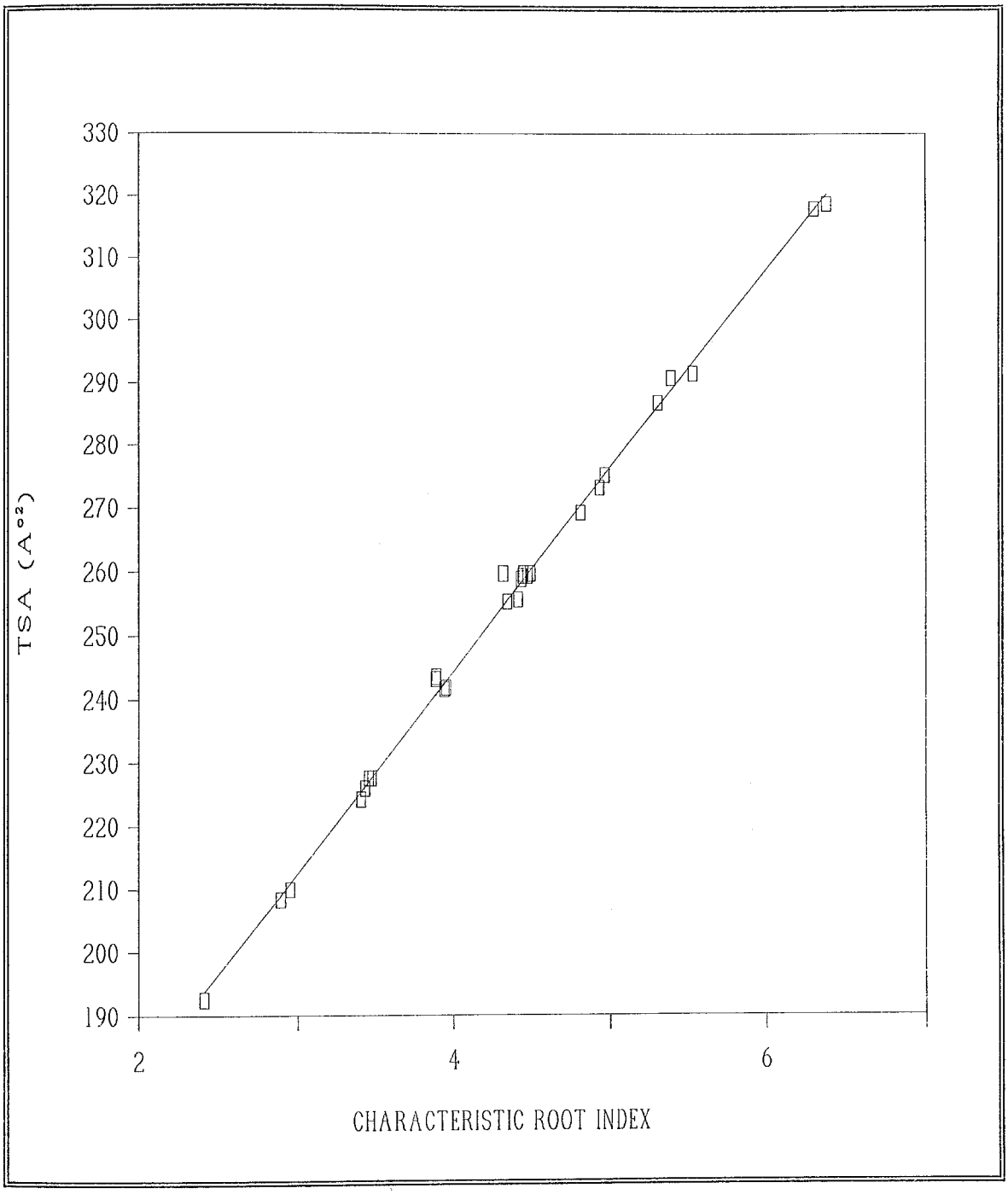


Figure 5.2. The total surface areas plotted as a function of the characteristic root indices of 27 PCBs from Table 5.2. and Ref.48.

Table 5.3. PHYSICOCHEMICAL PROPERTIES OF INDIVIDUAL CHLORINATED BIPHENYLS

COMPOUND	Log S (mol/l)	Log K_{OW}	Log P (mmHg)
BIPHENYL	-4.34 46,48 -4.33 47,48 -4.36 47,54 -4.40 49 -4.31 47,48,56 -4.25 50 -4.41 48,95 -4.60 48 -3.88* 61,57	4.09 57,72 3.90 75 3.89 47,65 3.76 47,54 3.75 47,50 4.03 50 4.10 70 4.17 58 4.04 47,64,74 3.87 56	-2.112 78 -2.014 78 -2.362 78 -2.138 78 -2.120 79 -1.304 77 -1.376 77 -2.044 78
2-CHLORO	-4.65 45,47,48 -4.57 47,54,55 -4.50 45,48 -4.57 47,54 -4.51 48 -4.65 47 -4.57* 62,57	4.59 5,70,71 4.51 71 4.30 75 4.50 54,62 4.38 70,71 4.80 70 3.75 70 4.60 35 4.54 57	-1.186 77 -1.782 77 -2.075 35 -1.940 79
4-	-5.05 56 -5.32 45,48 -7.09 45 -5.20 45,48 -5.16 45 -5.67 45 -5.00 48 -5.19 55	4.69 70 4.49 65,70,71 4.61 70,71 4.80 70 4.34 70 4.25 67 4.89 56	-2.075 59 -2.346 58 -2.880 78,79 -2.156 77 -2.167 77 -2.339 77
2-2'-DICHLORO	-5.45 45,48 -7.02 45 -5.39 45 -5.17 45,48 -5.34 45,48 -5.30 55	5.00 5,70,71 4.90 65,71 5.51 70 3.55 70 5.02 70 4.04 67 4.80 62,71	-2.571 58 -2.650 77 -2.997 79
4-4'-	-6.60 45,48 -6.44 45,48 -6.55 48,51,56 -6.33 48	5.33 65 5.36 70,71 5.58 51,68,70 5.51 70,71 4.92 70 5.28 70 5.17 67 5.49 76 5.57 56	-4.700 79 -3.237 77 -3.485 77

Table 5.3. CONTINUED

COMPOUND	Log S (mol/l)	Log K_{ow}	Log P (mmHg)
2-5-	-5.58 45,48,47 -6.04 45 -5.06 45,47 -5.04 51 -5.82 47 -5.02 48	5.10 75 5.16 54 5.18 71	-3.230 79 -2.860 77 -3.237 77
2-6-	-5.61 45 -5.20 47,54 -5.18 51 -5.82 47	5.00 75 4.93 54	
2-4'-	-5.55 45,48 -6.20 45,48 -5.54 45,48 -5.07 45,48 -5.22 48 -5.28* 62 -5.32* 61	5.14 64,71 5.10 62,63,72 5.14 65 5.64 70 6.22 70 4.34 70	-2.699 83
3-4-		5.51 70 5.29 65 5.10 70	
3-3'-			-3.710 79
2-2'-4-		5.76 75	
2-2'-3-		5.31 75	
2-2'-5-	-6.62 45 -5.60 45 -6.01 45 -6.03 55	5.55 75 5.60 65,69,70 6.22 70 4.34 70 5.58 56	-2.823 59 -2.698 55
2-3-4'-		5.42 75	
2-4'-5-	-6.45 45 -7.36 58	5.69 75 5.60 69 5.11 71 5.77 71 5.79 71 4.96 59 5.56 73 6.19 76	-3.520 77

Table 5.3. CONTINUED

COMPOUND	Log S (mol/l)	Log K_{OW}	Log P (mmHg)
2-3-3'-		5.57 [75]	
3-4-4'-		4.94 [75] 5.90 [71]	
2-4-4'-	-6.58 [45] -5.99 [45,48] -6.48 [45,48,56] -5.98 [48] -5.98* [62]	5.74 [71] 5.69 [75] 5.58 [65] 5.62 [62,71]	
2-4-5-	-6.44 [45,48] -6.20 [47,54] -6.33 [47] -6.12 [48]	5.60 [71] 5.79 [65] 5.81 [47,51] 5.51 [54] 6.22 [70] 5.86 [70] 5.77 [70]	-3.478 [77]
2-4-6-	-6.05 [47] -6.05 [47,54] -6.33 [47]	5.50 [75] 5.57 [65] 5.47 [54]	-4.031 [79] -3.056 [77] -3.648 [77]
2-2'-3-4-		6.11 [75]	
2-2'-3-5'-	-6.23 [45]	5.81 [75]	
2-2'-4-4'-	-6.63 [45] -6.73 [45] -7.23 [56]	6.29 [75] 5.68 [71] 6.11 [56]	
2-3-4-4'-		5.84 [75]	
2-2'-5-5'-	-7.28 [45] -6.59 [45] -7.03 [47] -7.11 [45] -7.04 [45,48] -6.80 [45,48] -7.68 [45,48] -6.58* [61] -7.05 [55]	6.11 [56] 6.09 [75] 5.90 [63,69] 6.26 [71] 5.81 [72]	-4.300 [79] -4.430 [80] -3.720 [80] -3.844 [77] -4.108 [77] -3.107 [55]
2-3'-4-4'-	-6.70 [45] -7.24 [48]	6.31 [75]	-4.335 [77]
2-3'-4'-5-	-7.26 [45] -6.85 [45,48] -7.00 [48]	6.39 [71] 6.23 [75] 5.95 [71]	-4.353 [77]
2-2'-3-3'-	-6.93 [45,48] -7.04 [48]		-4.134 [77]

Table 5.3. CONTINUED

COMPOUND	Log S (mol/l)	Log K_{OW}	Log P (mmHg)
3-3'-4-4'-	-8.70 [52] -8.59 [52] -7.98 [53] -7.22 [48] -8.59 [45] -6.22 [45] -8.21 [45] -7.16 [55]	6.04 [67]	-4.809 [77]
2-3-5-6-		5.46 [67]	
2-4-4'-5-		6.67 [67]	
2-3-4-5-	-7.18 [45,48] -7.14 [47,54] -6.73 [47] -6.74 [48] -7.18 [47]	5.91 [75] 5.72 [54]	
2-2'-5-6'-		5.90 [69]	-3.688 [77]
2-2'-4-5-	-4.24 [54] -6.73 [47]	5.73 [54,75] 6.22 [75]	
2-3'-4-4'-5-		7.12 [75]	-5.047 [77]
2-3-3'-4-4'-			-5.170 [77]
2-3-4-5-6-	-7.38 [45] -7.68 [45,47,48] -7.70 [45,48] -7.77 [47,54] -7.19 [47] -7.55 [48]	6.30 [54,75]	
2-2'-3-4-4'-		6.61 [64]	
2-2'-3-5'-6-		6.55 [64]	
2-2'-3-4-5'-	-7.86 [45] -7.15 [45]	6.37 [75] 6.85 [71]	-4.770 [77]
2-2'-3'-4-5-		6.67 [75]	
2-2'-4-4'-5-		7.21 [75]	-4.658 [77]
2-2'-4-5-5'-	-7.32 [52] -7.22 [47] -7.88 [47,48,52] -7.45 [53] -7.30 [48] -7.51 [45,47,56] -7.02 [45,48] -7.43 [52] -7.19 [47]	7.07 [75] 6.50 [65] 5.92 [47] 6.11 [51,68,70] 6.44 [47] 6.85 [70,71] 7.64 [70] 6.30 [56]	-5.140 [80] -5.080 [80] -5.070 [79] -4.560 [77] -4.620 [77]
2-3-3'-4'-6-		5.62 [75]	

Table 5.3. CONTINUED

COMPOUND	Log S (mol/l)	Log K_{OW}	Log P (mmHg)
22'-33'-66'-	-7.77 [47,54] -7.90 [52] -8.23 [53] -8.04 [52] -7.56 [45,47]	6.70 [75] 6.00 [73] 6.81 [65] 6.63 [54]	-6.660 [79]
22'-3-44'-5-		7.44 [75]	-5.397 [77]
22'-3-4-55'-		7.59 [75]	
22'-3-4'-55'-		7.31 [75]	
22'-44'-55'-	-7.85 [45] -8.57 [45,51] -8.11 [48] -8.53 [45,48] -7.61 [45,48] -8.47 [45,48] -7.56 [48] -8.55 [56] -7.66* [61]	7.75 [64] 6.90 [65] 7.44 [70] 6.72 [51,68,70] 8.35 [70,71] 6.56 [56] 6.34 [5] 8.18 [5]	-5.280 [77]
22'-33'-44'-	-7.56 [5,45,47] -9.11 [5] -8.91 [45,47,48] -8.43 [48] -9.10 [47]	7.00 [75] 6.96 [75] 6.93 [75] 7.44 [75]	-5.592 [77]
22'-44'-66'-	-8.94 [47,54] -7.56 [47] -8.24 [48] -8.60 [45,47] -8.51 [45]	7.55 [54,64] 7.00 [75] 6.10 [73]	-4.880 [79]
22'-33'-44'-6-	-8.26 [47,54] -7.80 [45,47] -8.26 [47]	6.68 [54]	-5.752 [77]
22'-33'-44'-55'-	-9.53 [45] -8.77 [45] -8.15 [45] -9.62 [48] -9.19 [48] -7.77 [48]		
22'-33'-55'-66'-	-9.46 [52] -9.03 [47,54] -9.37 [45,47,52] -9.40 [53] -9.68 [47,48]	7.14 [70] 7.10 [75] 7.21 [65] 7.11 [54] 9.77 [70] 8.42 [70]	-6.662 [78] -5.306 [77]

The superscripts are the references. The numbers with the stars are supercooled solute solubilities reported in the literature.

5.2. CORRELATIONS TO PHYSICOCHEMICAL PROPERTIES

5.2.1. WATER SOLUBILITY

The solubility of pollutants in water is of central importance in environmental science, and the calculation of solubility from structural and other parameters is a subject of considerable current interest. Polychlorinated biphenyls (PCBs) are mixtures of a large number of individual compounds that are widely distributed in the environment. Their transport through the environment is controlled by the solubility, vapour pressure and octanol-water partition coefficients of the individual compounds in the mixtures. The earliest solubility data on PCBs are aqueous solubilities of commercial mixtures. A considerable volume of data has been published on PCB isomer solubility[45], but discrepancies exist because of the experimental difficulty of generating and handling such dilute solutions. One of the objectives of this work is to gather the available data, and suggest a correlation which can be used to predict solubilities for PCB congeners for which no experimental data exist. It is recognized that correlations can be very valuable to obtain solubility data.

In general, physicochemical properties of solids are functions of molecular size and melting point, whereas for liquids and subcooled liquids they are functions of molecular size only[85]. PCBs are mostly solids but they occur in the environment only as mixtures of subcooled liquids. Therefore to identify any possible relationship with the CR index, subcooled liquid values are most appropriate for solid (mp > 25°C) congeners. All solid solubilities are converted into

subcooled liquid values by using the melting point of the congener of interest and the following equation

$$S_L = S_S \exp\left(-6.79\left(1 - \frac{T_m}{T}\right)\right) \qquad (5.2)$$

where, S_S is the solid solubility (mol/l), S_L is the subcooled liquid solubility, T_m is the melting point (°C), and T is the system temperature (25°C).

Table 5.4. gives selected experimental aqueous solubilities and melting points for the congeners and calculated subcooled liquid solubilities using equation (5.2). The correlation with the CR index, which is also shown as a line in Fig.5.3. is determined by linear regression and is

$$\text{Log}\, S_L = -1.197\ \text{CRI} - 1.126 \qquad (5.3)$$

$$n = 32;\quad r^2 = 0.972;\quad r = 0.985;\quad S_{y,x} = 0.197$$

with a correlation coefficient equal to 0.985. It allows estimation to within a factor of 1.57, which is sufficient for environmental fate determination[85]. So the present correlation shows that the CR index can be used for the rapid estimation of solubility of PCB congeners.

5.2.2. VAPOUR PRESSURE

Volatility is an important factor governing the transport of organics. Evaporation of industrial compounds such as PCBs from disposal sites depends on vapour pressure, and their ultimate return to the earth is also controlled by volatility. Vapour pressures have been accurately determined for many types of high molecular weight organics including insecticides and herbicides, phthalate esters, polycyclic aromatics[80]. Only

Table 5.4. LITERATURE AND CORRELATED SOLUBILITY DATA FOR PCB CONGENERS

COMPOUND	MELTING POINT	LogS	$LogS_L$	$LogS_L$ (PREDICTED)
BIPHENYL	71.00	-4.310	-3.900	-4.010
2-CHLORO	34.00	-4.570	-4.624	-4.590
4-	77.70	-5.003	-4.570	-4.661
2-2'-DICHLORO	61.00	-5.450	-5.092	-5.204
4-4'-	149.00	-6.330	-5.780	-5.286
2-5-	23.00	-5.600	-5.046	-5.263
2-6-	34.90	-5.630	-5.194	-5.241
2-4'-	43.00	-5.550	-5.375	-5.235
3-4-	29.00			-5.230
3-3'-				-5.253
2-2'-4-				-5.836
2-2'-3-				-5.852
2-2'-5-	44.00	-6.023	-5.807	-5.858
2-3-4'-				-5.872
2-4'-5-	64.000	-6.369	-5.996	-5.833
2-3-3'-				-5.824
3-4-4'-	88.00			-5.778
2-4-4'-	57.00	-5.990	-5.655	-5.783
2-4-5-	78.00	-6.199	-5.772	-5.831
2-4-6-	62.00	-6.330	-5.966	-5.846
2-2'-3-4-				-6.422
2-2'-3-5'-		-6.230	-5.977	-6.470
2-2'-4-4'-	42.00	-6.730	-6.545	-6.452
2-3-4-4'-				-6.296
2-2'-5-5'-	87.00	-7.060	-6.609	-6.507
2-3'-4-4'-	128.00	-6.910	-6.387	-6.444
2-3'-4'-5-	104.00	-6.852	-6.365	-6.485
2-2'-3-3'-	121.00	-6.930	-6.416	-6.412

Table 5.4. CONTINUED

COMPOUND	MELTING POINT	LogS	$LogS_L$	$LogS_L$ (PREDICTED)
3-3'-4-4'-	180.00	-7.220	-6.647	-6.435
2-3-5-6-				-6.139
2-4-4'-5-				-6.415
2-3-4-5-	92.00	-6.741	-6.278	-6.331
2-2'-5-6'-				-6.486
2-2-'6-6'-				-6.417
2-2'-4-5-	66.10	-6.737	-6.355	-6.467
2-3'-4-4'-5-				-7.012
2-3-3'4-4'-				-6.990
2-3-4-5-6-	124.00	-7.380	-6.862	-6.893
2-2'3-4-4'-				-6.998
2-2'3-5'-6-				-7.060
2-2'-4-6-6'-				-7.036
2-2'-3-4-5'-	112.00	-7.860	-7.360	-7.039
2-2'-3'-4-5-				-6.981
2-2'-4-4'-5-				-7.030
2-2'-4-5-5'-	77.00	-7.489	-7.066	-7.079
2-3-3'-4'-6-				-6.985
2-2'-3-4-4'-5-				-7.495
2-2'-3-3'-6-6'-	112.20	-8.045	-7.545	-7.591
2-2'-3-4-5-5'-				-7.593
2-2'-3-4'-5-5'-				-7.579
2-2'-4-4'-5-5'-	103.00	-8.110	-7.625	-7.585
2-2'-4-5-5'-6-				-7.650
2-2'-3-3'-4-4'-	150.00	-8.436	-7.889	-7.486
2-2'-4-4'-6-6'-	114.00	-8.240	-7.736	-7.753
22'-33'-44'-6-	122.40	-8.260	-7.744	-8.127
22'-33'-44'-55'-	159.00	-9.190	-8.634	-8.673
22'-33'-45'-66'-				-8.773
22'-33'-55'-66'-	162.00	-9.380	-8.822	-8.768

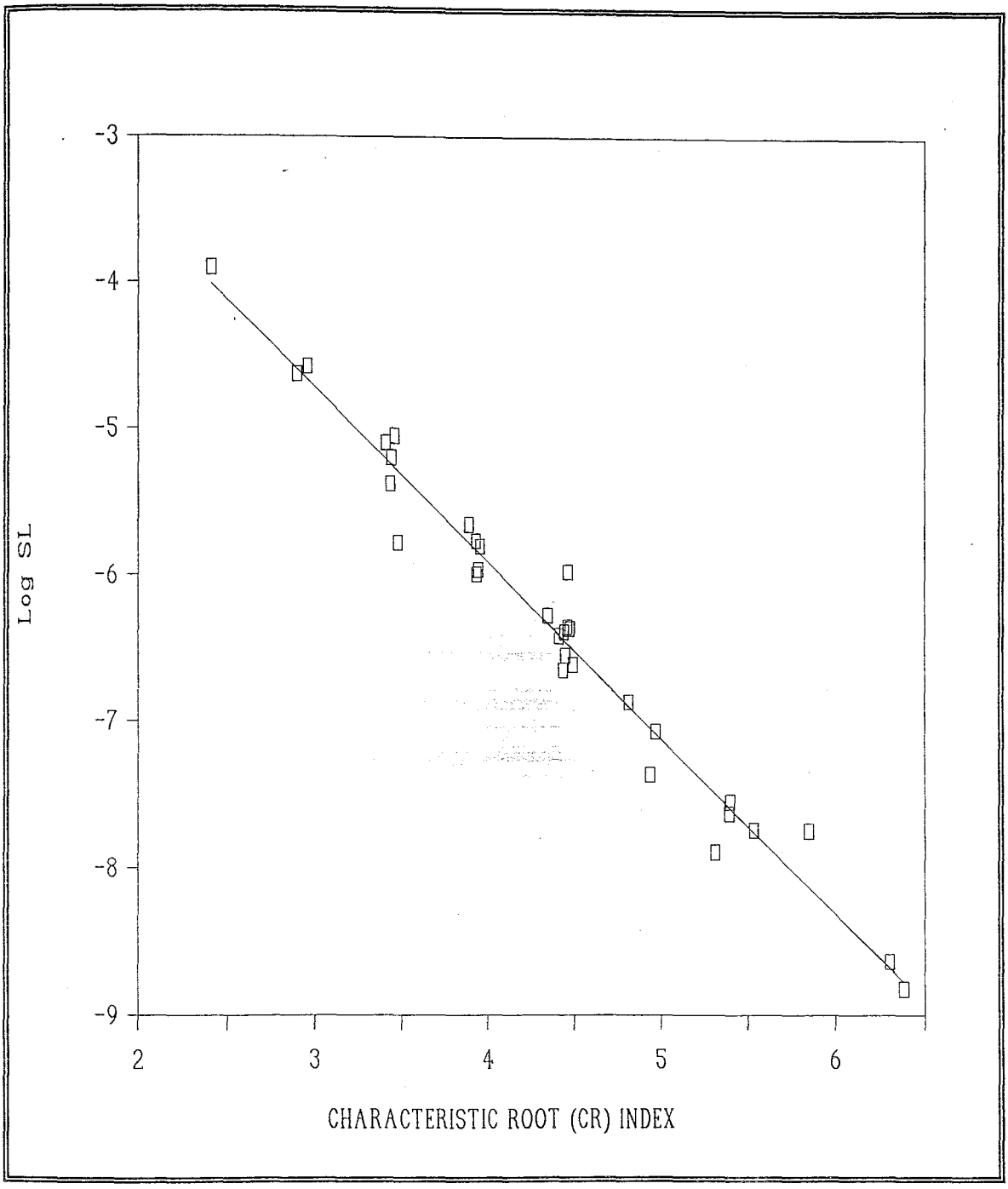


Figure 5.3. Relationship between subcooled liquid solubility of PCBs and characteristic root index .

limited vapour pressure data are available for PCBs, an important class of organic pollutants. Up to a few years ago, the only vapour pressure information available was for Aroclor fluids, determined in the 150 - 300°C range by Monsento Corporation(77). Mackay and Wolkoff extrapolated these data to estimate Aroclor vapour pressures at 25°C , which today are the most widely quoted volatility data for PCB fluids. Aroclor mixtures contain fifty or more components and the vapour pressures referenced above are dominated by a few of the more volatile PCBs.

Of the 209 possible PCBs, vapour pressures of only a few have been directly measured by physical methods (effusion, gas saturation, or extrapolation from boiling point data). Recently, Biddleman(77), estimated the liquid phase vapour pressures (P_L) at 25°C of 30 PCBs using capillary gas chromatographic (GC) method. In the present work, most of the vapour pressure data have been taken from Biddleman(77) to estimate the liquid phase vapour pressures of 58 PCB congeners. Linear regression of vapour pressure values against CR index results in

$$\text{Log}P = - 1.332\ CRI + 1.706 \qquad (5.4)$$

$$n = 31;\quad r^2 = 0.908;\quad r = 0.952;\quad S_{y,x} = 0.4$$

The average difference between predicted and observed vapour pressures is only 0.4 log unit (factor of 2.51). Table 5.5. gives the used experimental and predicted vapour pressures of PCB congeners by using regression equation (5.4). The regression line for PCBs is shown in Fig.5.4.

Table 5.5. LITERATURE AND CORRELATED VAPOUR PRESSURES OF PCBs.

COMPOUND	Log P (Observed)	Log P (Predicted)
BIPHENYL	-1.376	-1.504
2-CHLORO	-1.940	-2.150
4-	-2.156	-2.230
2-2'-DICHLORO	-2.650	-2.834
4-4'-	-3.237	-2.924
2-5-	-2.860	-2.899
2-6-		-2.875
2-4'-	-2.699	-2.869
3-4-		-2.863
3-3'-	-3.710	-2.889
2-2'-4-TRICHLORO		-3.535
2-2'-3-		-3.555
2-2'-5-	-2.824	-3.562
2-3-4'-		-3.577
2-4'-5-	-3.520	-3.534
2-3-3'-		-3.525
3-4-4'-		-3.473
2-4-4'-		-3.479
2-4-5-	-3.478	-3.532
2-4-6-	-3.648	-3.549
2-2'-3-4-TETRACHLORO		-4.189
2-2'-3-5'-		-4.244
2-2'-4-4'-	-4.066	-4.224
2-3-4-4'-		-4.050
2-2'-5-5'-	-4.300	-4.284
2-3'-4-4'-	-4.335	-4.214
2-3'-4'-5-	-4.353	-4.259
2-2'-3-3'-	-4.134	-4.179

Table 5.5. CONTINUED

COMPOUND	Log P (Observed)	Log P (Predicted)
3-3'-4-4'-	-4.809	-4.205
2-3-5-6-		-3.875
2-4-4'-5-		-4.182
2-3-4-5-		-4.088
2-2'-5-6'-	-3.688	-4.261
2-2-'6-6'-		-4.184
2-2'-4-5-		-4.240
2-3'-4-4'-5-PENTACHLORO	-5.047	-4.846
2-3-3'4-4'-	-5.170	-4.822
2-3-4-5-6-		-4.714
2-2'3-4-4'-		-4.832
2-2'3-5'-6-		-4.900
2-2'-4-6-6'-		-4.873
2-2'-3-4-5'-	-4.770	-4.877
2-2'-3'-4-5-		-4.813
2-2'-4-4'-5-	-4.685	-4.867
2-2'-4-5-5'-	-5.079	-4.921
2-3-3'-4'-6-		-4.816
2-2'-3-4-4'-5-HEXACHLORO	-5.397	-5.385
2-2'-3-3'-6-6'-	-6.660	-5.491
2-2'-3-4-5-5'-		-5.493
2-2'-3-4'-5-5'-		-5.478
2-2'-4-4'-5-5'-	-5.280	-5.485
2-2'-4-5-5'-6-		-5.557
2-2'-3-3'-4-4'-	-5.592	-5.375
2-2'-4-4'-6-6'-	-4.880	-5.671
2-2'-3-3'-4-4'-6-HEPTACHLORO	-5.752	-6.088
2-2'-3-3'-4-4'-5-5'-OCTACHLORO		-6.696
2-2'-3-3'-4-5'-6-6'-		-6.807
2-2'-3-3'-5-5'-6-6'-	-6.662	-6.802

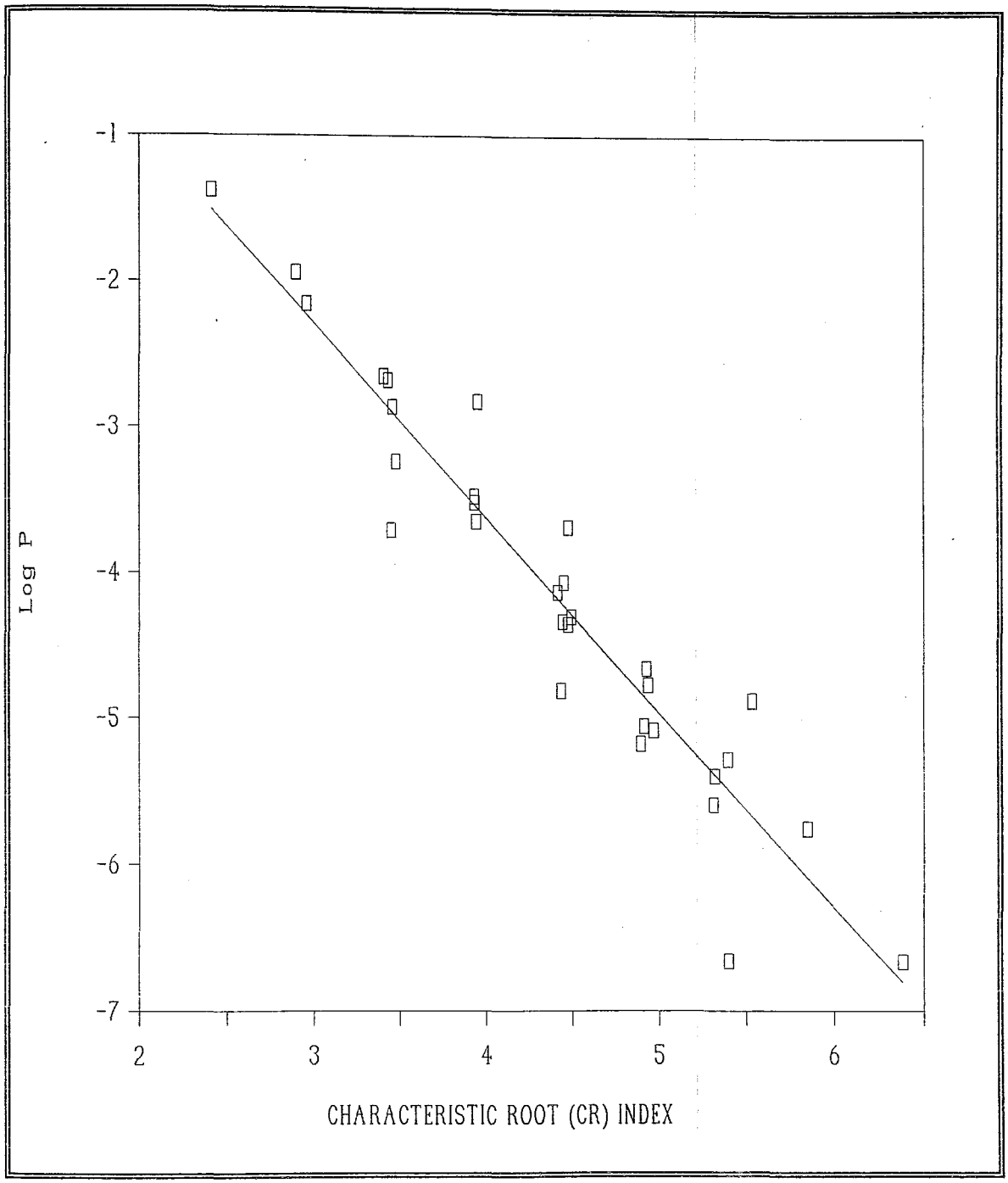


Figure 5.4. Relationship between vapour pressure and characteristic root index of PCBs.

5.2.3. OCTANOL WATER PARTITION COEFFICIENT

The n-octanol/water partition coefficient has proved useful as a means to predict soil adsorption, biological uptake, and biomagnification[51]. By definition, the partition coefficient expresses the equilibrium concentration ratio of an organic chemical partitioned between an organic liquid (e.g., n-octanol) and water. This partitioning is , in essence, equivalent to partitioning an organic chemical between itself and water.

Partition Coefficient (K_{ow}) chemical in organic solvent ⇔ aqueous solution

It has been linearly related to fish bioconcentration factors, to soil organic carbon partition coefficients, and to toxicities to a wide variety of aquatic and mammalian species. PCBs display appreciable partitioning into organic media as a result of their low solubility, or correspondingly their large K_{OW} values. In view of the large number of chemical species, and the difficulty of experimental measurements, there is an incentive to develop a methodology for prediction of Log K_{OW} values based only on a knowledge of chemical structures.

The literature K_{OW} values, however, are often not experimental, but rather calculated. Lyman et al[75], have summarized the methods that are commonly used for the estimation of K_{OW}.

In this work, reported experimental and calculated K_{OW} values were used. Single K_{OW} values which were either estimated or calculated were not included in the correlations. When more than one reported experimental or calculated octanol-water partition coefficient value was available, either one of them

was selected or their average was included in the regression, if they were close to each other.

Linear regression of Log K_{ow} for the selected data against the CR index showed a significant relationship expressed by

$$\text{Log } K_{ow} = 1.138 \text{ CRI} + 1.127 \qquad (5.5)$$

$$n = 32; \quad r^2 = 0.971; \quad r = 0.985; \quad S_{y,x} = 0.171$$

The agreement between estimated and literature values of K_{ow} was good, generally agreeing within a factor of 1.48 (or 0.17 log units). A plot of these data is shown in Fig.5.5. with the linear regression equation (5.5) represented by the solid line. Table 5.6. tabulates the selected and calculated K_{ow} values for PCB congeners.

5.2.4. SOIL SORPTION COEFFICIENT

The soil sorption coefficient (K_{OC}), defined as the ratio between concentrations of a given chemical sorbed by the soil and dissolved in the soil water normalized to the total organic carbon content of the soil, is currently used as a quantitative measure of soil sorption[4].

Soil Adsorption K_D chemical adsorbed on soil $\Leftrightarrow$ aqueous solution

$$K_{oc} = \frac{100 K_D}{\%\ \text{organic carbon}}$$

The experimental determination of K_{OC} values is often costly and time consuming process. It is also very inaccurate for

Table 5.6. LITERATURE AND CORRELATED OCTANOL WATER PARTITION COEFFICIENTS OF PCBs.

COMPOUND	Log K_{OW} (Observed)	Log K_{OW} (Predicted)
BIPHENYL	3.886	3.870
2-CHLORO	4.340	4.421
4-	4.490	4.489
2-2'-DICHLORO	5.010	5.005
4-4'-	4.920	5.083
2-5-	5.106	5.061
2-6-	4.965	5.040
2-4'-	5.126	5.035
3-3'-		5.051
3-4-	5.100	5.030
2-2'-4-TRICHLORO		5.606
2-2'-3-		5.621
2-2'-5-	5.570	5.627
2-3-4'-		5.640
2-4'-5-	5.580	5.603
2-3-3'-		5.595
3-4-4'-	5.900	5.551
2-4-4'-	5.580	5.556
2-4-5-	5.540	5.602
2-4-6-	5.600	5.616
2-2'-3-4-TETRACHLORO		6.163
2-2'-3-5-		6.209
2-2'-4-4'-	6.109	6.192
2-3-4-4'-	5.840	6.044
2-2'-5-5'-	6.260	6.244
2-3'-4-4'-		6.184
2-3'-4'-5-	6.230	6.223
3-3'-4-4'-	6.210	6.176
2-3-5-6-	5.940	5.894
2-4-4'-5-		6.156
2-3-4-5-	6.180	6.076
2-2'-3-3'-		6.154

Table 5.6. CONTINUED.

COMPOUND	Log K_{OW} (Observed)	Log K_{OW} (Predicted)
2-2'-6-6'-		6.159
2-2'-5-6'-	5.900	6.224
2-2'-4-5-	6.220	6.207
2-2'-4-6-6'-PENTACHLORO		6.747
2-3'-4-4'-5-		6.724
2-3-3'-4-4'-		6.704
2-3-4-5-6-		6.611
2-2'-3-4-4'-		6.712
2-2'-3-5'-6-		6.770
2-2'-3-4-5'-	6.850	6.750
2-2'-3'-4-5-		6.695
2-2'-4-4'-5-	7.210	6.741
2-2'-4-5-5'-	6.850	6.788
2-3-3'-4'-6-		6.698
2-2'-4-5-5'-6-HEXACHLORO		7.331
2-2'-3-3'-6-6'-	6.810	7.275
2-2'-3-4-4'-5-		7.184
2-2'-3-4-5-5'-		7.277
2-2'-3-4'-5-5'-		7.264
2-2'-4-4'-5-5'-	7.440	7.270
2-2'-3-3'-4-4'-	6.960	7.176
2-2'-4-4'-6-6'-	7.550	7.429
2-2'-3-3'-4-4'-6-HEPTACHLORO		7.176
2-2'-3-3'-4-4'-5-5'-OCTACHLORO		9.304
2-2'-3-3'-4-5'-6-6'-		8.399
2-2'-3-3'-5-5'-6-6'-	8.420	8.395

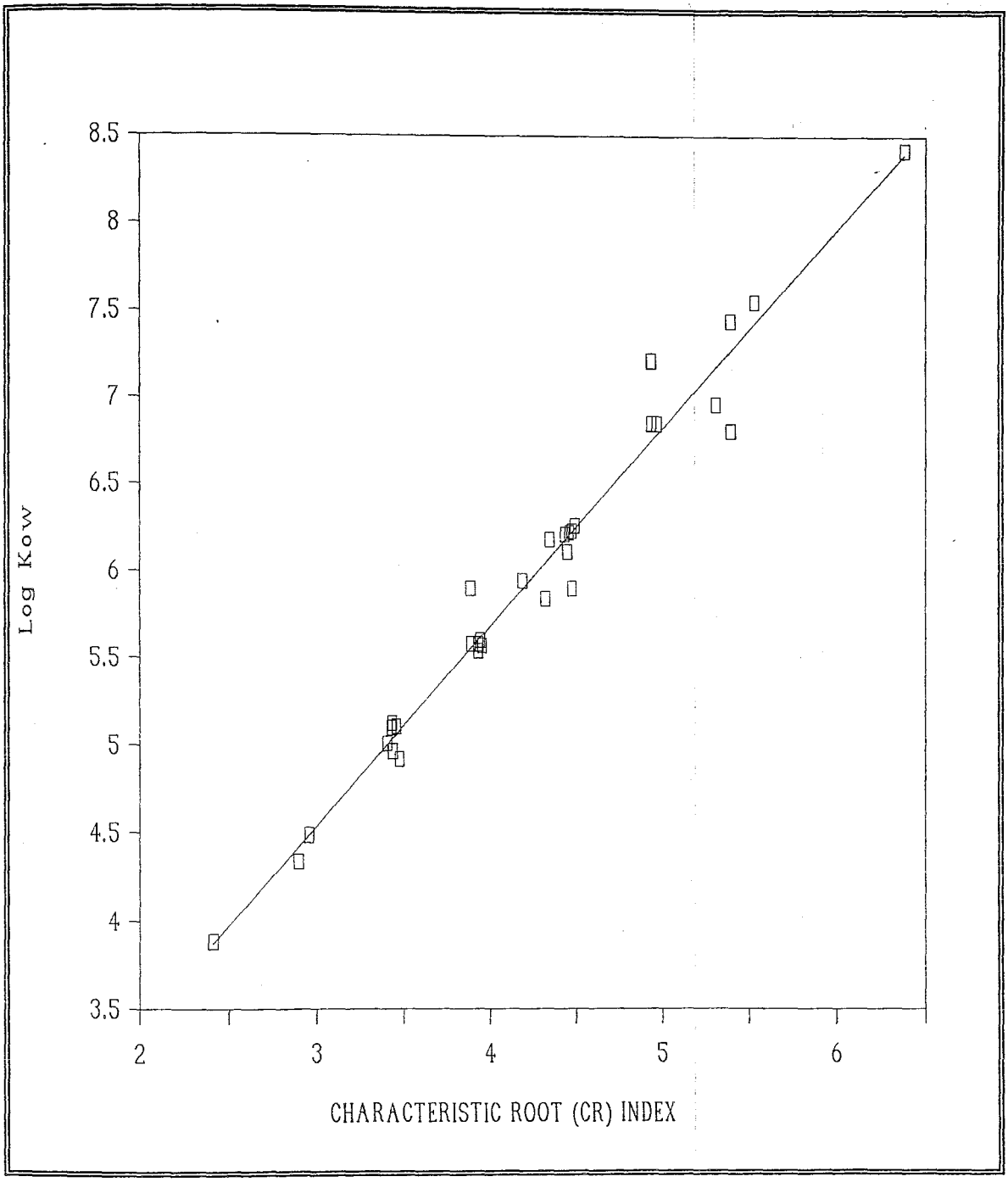


Figure 5.5. Relationship between octanol-water partition coefficient of PCBs and characteristic root index.

compounds with low water solubility, such as PCBs. Thus a convenient, accurate way to predict soil sorption coefficients of PCBs is needed.

In this investigation, molecular topology and QSAR analysis have been applied to this problem, with the aim of finding a structural parameter that will describe the relationship between the molecular structure of PCBs and their adsorption by soil. However, only 9 K_{OC} values of PCBs are reported in the literature. The CR index was used to correlate with these 9 soil sorption coefficients. The following linear relationship was established between the CR index and Log K_{OC}.

$$\text{Log}K_{oc} = 0.689\ CRI + 1.410 \qquad (5.6)$$

$n = 9;\quad r^2 = 0.904;\quad r = 0.941;\quad S_{y,x} = 0.222;$

On the other hand, in numerous studies involving a wide variety of chemicals, the correlation between K_{OW} and K_{OC} has been examined[89]. Published equations "calibrated" on sets of hydrophobic compounds include the following:

$$\text{Log}K_{oc} = 1.029\,\text{Log}K_{ow} - 0.18 \quad (13\ \text{pesticides},\ r^2 = 0.91)^{(89)} \qquad (5.7)$$

$$\text{Log}K_{oc} = 0.989\,\text{Log}K_{ow} - 0.356 \quad (5\ \text{PNAs},\ r^2 = 0.997)^{(90)} \qquad (5.8)$$

$$\text{Log}K_{oc} = \text{Log}K_{ow} - 0.32 \quad (n = 22,\ r^2 = 0.98)^{(89)} \qquad (5.9)$$

$$\text{Log}K_{oc} = 0.54\,\text{Log}K_{ow} + 0.76 \quad (n = 10,\ r^2 = 0.96)^{(88)} \qquad (5.10)$$

$$\text{Log}K_{oc} = 0.54\,\text{Log}K_{ow} + 0.64 \quad (n = 105,\ r^2 = 0.95)^{(88)} \qquad (5.11)$$

$$\text{Log}K_{oc} = 1.00\,\text{Log}K_{ow} - 0.21 \quad (n = 10,\ r^2 = 1)^{(91)} \qquad (5.12)$$

In order to find a better correlation for soil sorption coefficients of PCBs, an analogous regression analysis with K_{ow} values was carried out, resulting in the linear regression equation:

$$\text{Log}\,K_{oc} = 0.594\ \text{Log}\,K_{ow} + 0.78 \qquad (5.13)$$

$$n = 9;\quad r^2 = 0.904;\quad r = 0.941,\quad S_{y,x} = 0.222$$

for which the correlation coefficient was 0.941. On the other hand eq.(5.13) is almost identical with the equation reported by Briggs[88] [eq. (5.10)]. Calculated soil sorption coefficients of PCBs using eq.(5.6) and eq. (5.13) were compared with the experimental K_{OC} values reported by Sabljic[4]. Calculated K_{OC} values obtained from eq.(5.13) were closer to the experimental K_{OC} values. So, in the prediction of K_{OC} values eq.(5.13) was used. Table 5.7. includes the data taken from Sabljic[4] and predicted K_{OC} values obtained from eq.(5.13).

5.2.5. HENRY's LAW CONSTANT

One of the major problems in modelling and predicting the behaviour of PCBs in the environment has been the lack of accurate Henry's Law Constants (HLC). They are used to predict exchange rates of vapours across the air/ water interface and fugacity potentials for aqueous systems.

In part, HLCs have not been available due to analytical difficulties in measuring this property. The quantity of available data are insufficient. Recently Dunnivat[92], reported experimental HLCs for several PCBs . Linear regression of Log HLC (atm m^3/mol) for the experimental data , however, results in a much poorer correlation with the CR index.

Table 5.7 PREDICTED[1] AND EXPERIMENTAL VALUES OF K_{OC} REPORTED BY SABLJIC[4]

COMPOUND	Log K_{OC} EXPERIMENTAL[4]	Log K_{OC} PREDICTED[a]	Log K_{OC} PREDICTED[b]
BIPHENYL		3.090	3.081
2-CHLORO	3.230	3.360	3.408
4-		3.449	3.449
2-2'-DICHLORO	3.680	3.758	3.755
4-4'-		3.705	3.802
2-5-		3.816	3.789
2-6-		3.732	3.776
2-4'-	3.890	3.827	3.773
3-4-		3.812	3.770
3-3'-			3.783
2-2'-4-			4.113
2-2'-3-			4.122
2-2'-5-		4.091	4.125
2-3-4'-			4.133
2-4'-5-		4.097	4.111
2-3-3'-			4.106
3-4-4'-		4.288	4.080
2-4-4'-	4.380	4.097	4.083
2-4-5-		4.074	4.110
2-4-6-		4.109	4.119
2-2'-3-4-			4.444
2-2'-3-5'-			4.471
2-2'-4-4'-		4.412	4.461
2-3-4-4'-		4.252	4.373
2-2'-5-5'-	4.670	4.502	4.492
2-3'-4-4'-		4.472	4.456

1 (a) Predicted from experimental K_{OW} , (b) Predicted from estimated K_{OW} by using eq. 5.13

Table 5.7. Continued

COMPOUND	Log K_{OC} EXPERIMENTAL[4]	Log K_{OC} PREDICTED[a]	Log K_{OC} PREDICTED[b]
2-3'-4'-5-		4.484	4.480
2-2'-3-3'-			4.439
3-3'-4-4'-			4.452
2-3-5-6-		4.311	4.284
2-4-4'-5-			4.440
2-3-4-5-		4.454	4.392
2-2'-5-6'-		4.288	4.480
2-2-'6-6'-			4.441
2-2'-4-5-		4.478	4.470
2-3'-4-4'-5-			4.777
2-3-3'-4-4'-			4.765
2-3-4-5-6-			4.740
2-2'-3-4-4'-			4.770
2-2'-3-5'-6-			4.805
2-2'-4-6-6'-			4.791
2-2'-3-4-5'-	4.500	4.852	4.793
2-2'-3'-4-5-			4.760
2-2'-4-4'-5-		5.066	4.787
2-2'-4-5-5'-	4.630	4.852	4.815
2-3-3'-4'-6-			4.762
2-2'-3-4-4'-5-			5.051
2-2'-3-3'-6-6'-		4.828	5.105
2-2'-3-4-5-5'-			5.106
2-2'-3-4'-5-5'-			5.098
2-2'-4-4'-5-5'-	5.340	5.203	5.102
2-2'-4-5-5'-6-			5.138
2-2'-3-3'-4-4'-	5.050	4.918	5.016
2-2'-4-4'-6-6'-		5.268	5.196
2-2'-3-3'-4-4'-6-			5.046
2-2'-3-3'-4-4'-5-5'-			6.311
2-2'-3-3'-4-5'-6-6'-			5.773
2-2'-3-3'-5-5'-6-6'-		5.786	5.771

On the other hand, HLC may be regarded as an air/ water partition coefficient and is often derived from the ratio of P_L/S_L. It is generally accepted that HLCs derived in this manner break down when vapour pressures exceed $(0.5 - 1)\times 10^6$ Pa, aqueous solubilities exceed 1.6×10^3 mol/m^3 or both (85). Of the PCB congeners, biphenyl possesses one of the highest vapour pressures (approximately 4 Pa) and aqueous solubilities [4.5×10^{-2} mol/m^3](83). These values are clearly within the limits of applicability stated above. So, the HLC of each congener was calculated using solubility and vapour pressure data tabulated in Table 5.3. and 5.4. respectively. Table 5.7 contains the calculated and experimental values of HLCs of PCBs. It was noted that HLC decreases with increasing number of chlorine atoms. The data were in close agreement for congeners biphenyl, 4- chloro, 2-4-5- and 2-4-6-TCB, and 22′-55′-TCB. However, significant differences resulted for 2- chloro, 2-4′-DCB, 2-2′-5-TCB, 22′- 33′-66′ and 22′-44′-66′-HCB. They are also outlying literature HLC values for most of the PCBs. There is a wide range of the HLC data with a minimum around 20 Pa m^3/mol and a maximum of 130 Pa m^3/mol for the same congener (e.g.; 2-2′-5-TCB). These contrasting results can be attributed to the method of analyzing the data and difficulties in measuring total initial aqueous PCB concentrations. In addition, the commonly used aqueous phase stripping method for HLC determination may be inappropriate.

Burkhard et al(53) reported an increase in HLCs with an increasing number of ortho-chlorine substitutions within the same molecular class. In contrast, Burkhard et al(1) state that

Table 5.8. CALCULATED[1] AND LITERATURE[2] HENRY'S LAW CONSTANTS OF PCBs

COMPOUND	HLC Pa m^3/mol		
	Calc.[a]	Calc.[b]	LITERATURE HLC
BIPHENYL	44.55	42.75	41.34 [c] 30.40 [c] 66.27 [c]
2-CHLORO	64.40	36.73	74.58 [c]
4-	36.89	35.98	58.06 [c]
2-2'-DICHLORO		31.24	22.29 [c] 55.72 [d] 34.14 [d]
4-4'-	46.55	30.68	14.69 [d] 30.39 [d] 11.04 [d]
			20.16 [d]
2-5-	20.46	30.81	33.30 [d] 39.31 [d]
2-6-		30.96	96.66 [d]
2-4'-	63.23	30.97	
3-4-		31.02	20.77 [d] 9.60 [d]
3-3'-		30.82	23.60 [d] 13.57 [d]
2-2'-4-		26.48	
2-2'-3-		26.42	81.77 [c]
2-2'-5-	128.21	26.36	20.06 [c] 101.50 [c]
2-3-4'-		26.22	
2-4'-5-		26.54	20.26 [c] 94.13 [c]
2-3-3'-		26.54	81.77 [c]
3-4-4'-		26.91	84.21 [c]
2-4-4'-		26.85	
2-4-5-	26.23	26.54	
2-4-6-	27.72	26.41	37.28 [d] 65.75 [d]
2-2'-3-4-		22.80	
2-2'-3-5'-		22.44	24.32 [c] 79.24 [c]
2-2'-4-4'-	40.17	22.54	
2-3-4-4'-		23.49	
2-2'-5-5'-	27.16	22.24	14.10 [c] 22.29 [c] 53.70 [c]
2-3'-4-4'-		22.64	84.20 [c]
2-3'-4'-5-	13.70	22.44	20.26 [c]

1 (a) Calculated values of HLC by using experimental vapour pressure and solubility data, (b) Caculated values of HLC by using predicted vapour pressure and solubility data.

2 (c) Data taken from Ref.83, (d) Data taken from Ref.92.

Table 5.8. CONTINUED

COMPOUND	HLC Pa m^3/mol		
	Calc.[a]	Calc.[b]	LITERATURE HLC
2-2′-3-3′-		22.80	20.46 [d]
3-3′-4-4′-	9.18	22.64	
2-3-5-6-		24.48	
2-4-4′-5-		22.76	
2-3-4-5-		23.33	
2-2′-5-6′-		22.38	46.68 [d]
2-2-′6-6′-		22.80	14.99 [d] 39.00 [d] 188.45 [d]
2-2′-4-5-		22.47	
2-3′-4-4′-5-		19.53	
2-3-3′4-4′-		19.62	
2-3-4-5-6-		19.92	
2-2′3-4-4′-		19.54	
2-2′3-5′-6-		19.26	
2-2′-4-6-6′-		19.40	50.15 [d]
2-2′-3-4-5′-	51.87	19.36	33.44 [c]
2-2′-3′-4-5-		19.63	
2-2′-4-4′-5-		19.40	
2-2′-4-5-5′-	12.94	19.18	11.46 [c] 35.46 [c] 40.93 [d]
2-3-3′-4′-6-		19.67	
2-2′-3-4-4′-5-		17.17	40.64 [c]
2-2′-3-3′-6-6′-	1.02	16.74	
2-2′-3-4-5-5′-		16.78	
2-2′-3-4′-5-5′-		16.82	
2-2′-4-4′-5-5′-	29.50	16.78	12.46 [d] 17.93 [d] 35.46 [d]
2-2′-4-5-5′-6-		16.52	
2-2′-3-3′-4-4′-	26.42	17.21	50.66 [c] 55.72 [d] 6.84 [d]
2-2′-4-4′-6-6′-	95.70	16.10	15.70 [d] 76.49 [d] 84.60 [d]
22′-33′-44′-6-		14.58	
22′-33′-44′-55′-		12.64	
22′-33′-45′-66′-		12.32	
22′-33′-55′-66′-		12.33	

HLCs increase with decreasing ortho-chlorine substitution for each weight class. In addition, it was reported that congeners with the highest degree of meta- and/or para-chlorine substitution possessed the highest HLCs. In this study, this trend was not observed in the estimated values of HLCs. More HLC data and further development of QSAR models for PCB congeners are required for quantitative estimates of HLCs of PCBs. Also relationships of HLCs between molecular weight classes probably require additional factors, since there is no apparent trend in the literature data in Table 5.8. when all data are considered together. Although comparison of the experimental and calculated HLCs reveal fair agreement for several compounds, and the same trend appears in the literature values, calculated values of HLCs obtained from both experimental and predicted input data were used in the Model.

5.2.6. BIOCONCENTRATION FACTOR

A major problem in environmental contamination by pollutants is the extent that these pollutants may concentrate from water into aquatic organisms such as fish[72]. The extent of such concentration is expressed as the bioconcentration factor (K_B), i.e., by the ratio of the steady state concentration of a chemical in the organism to that in water. It has been generally assumed that the mechanism leading to the uptake of organic pollutants by organisms is analogous to the partitioning between an organic phase and water.

Bioconcentration factor (K_B) chemical in organism $\Leftrightarrow$ aqueous solution.

Hence, Log K_B values of organic compounds from both laboratory bioconcentration testing and natural water systems have been correlated either with the corresponding octanol-water partition coefficients or with their water solubilities[93,94].

Since there was lack of experimental bioaccumulation data for PCB isomers, they were obtained from the Mackay correlation[86] which is:

$$\text{Log}K_B = \text{Log}K_{ow} - 1.32 \qquad (5.14)$$

The relationship reported by Mackay between K_{OW} and bioconcentration factors for 71 chemicals, does include the bioaccumulation of several PCBs and has a high correlation coefficient (r=0.95), therefore it was used in Mackay's Level I Fugacity Model, by using both experimental and predicted Log K_{OW} values to estimate K_B of PCBs.

5.3. CALCULATION OF FUGACITY CAPACITY CONSTANTS IN TERMS OF EXPERIMENTAL AND PREDICTED INPUT DATA

The fugacity capacity (Z) values for a chemical can be estimated from the knowledge of vapour pressure, solubility and octanol-water partition coefficient. The formula of the fugacity capacity constants, Z_i, for each compartment of the environment described in Mackay's Model were given in Section IV. The procedure for the calculation of fugacity capacity constants for each compartment and for 4 - chloro biphenyl using experimental and predicted pyhsicochemical properties is given in the following peer section.

Specimen Calculation

5.3.1. CALCULATION OF THE FUGACITY CAPACITY CONSTANT FOR AIR

$$Z_A = \frac{1}{RT}$$

$T = 298°K$

$R = 8.314$ $(Pa.m^3/mol°K)$ or $(8.314$ $j/mol°K)$

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

As it can be seen from the formula the fugacity capacity constant for air is constant for all congeners.

5.3.2. FUGACITY CAPACITY CONSTANT FOR SOIL

$$Z_S = K_{p_s} \rho_s / HLC$$

5.3.2.1. Calculation of the Fugacity Capacity Constant, Z_S, for 4 - Chloro Biphenyl in terms of Experimental Input Data

$$HLC = \frac{P_L}{S_L} \quad Pa\ m^3/mole$$

$\log P_L = -2.156$ (from Table 5.5)

$P_L = 6.98 \times 10^{-3}$ mmHg

$$P_L = 6.98 \times 10^{-3} \text{ mmHg} \cdot \frac{1 \text{ Pa}}{7.5 \times 10^{-3} \text{ mmHg}}$$

$P_L = 0.930$ Pa

$\log S_L = -4.57$ (from Table 5.4)

$S_L = 2.69 \times 10^{-5}$ mol/litre

$$S_L = 2.69 \times 10^{-2} \text{ mol/m}^3$$

$$HLC = \frac{0.930}{2.69 \times 10^{-2}} = 34.59 \text{ Pa m}^3\text{/mol}$$

$$\text{Log } K_{oc} = 0.56 K_{ow} + 0.78$$

$$\text{Log } K_{oc} = 3.449$$

$$K_{oc} = 2811.9$$

K_{ps} = % organic carbon × K_{oc} m^3 of water/10^6g sorbent

$$K_{ps} = 0.02 \times 2811.9 \times 10^{-6}$$

$$K_{ps} = 56.24 \times 10-6$$

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

$$Z_s = 56.24 \times 10^{-6} \times 1.5 \times 10^6 / 34.59 \text{ mole/m}^3 \text{ Pa}$$

$$Z_s = 2.43 \text{ mole/m}^3\text{Pa}$$

5.3.2.2. Calculation of the Fugacity Capacity Constant, Z_S, for 4 - Chloro Biphenyl in terms of Predicted Input Data

$$\text{Log } P_L = -2.23 \quad \text{(from Table 5.5)}$$

$$P_L = 5.89 \times 10^{-3} \text{ mmHg}$$

$$\text{Log } S_L = -4.661$$

$$S_L = 2.18 \times 10^{-5} \text{ mol/l}$$

$$S_L = 2.18 \times 10^{-2} \text{ mol/m}^3$$

$$HLC = \frac{0.785}{2.18 \times 10^{-2}} = 35.96 \text{ Pa m}^3\text{/mole}$$

$$\text{Log } K_{oc} = 3.449 \quad \text{(from Table 5.7)}$$

$$K_{ps} = 0.02 \times 2811.9 \times 10^{-6}$$

$$K_{ps} = 56.24 \times 10^{-6}$$

$$Z_s = 56.24 \times 10^{-6} \times 1.5 \times 10^{6} / 35.96$$

$$Z_s = 2.33 \text{ mole/m}^3\text{Pa}$$

5.3.3. FUGACITY CAPACITY CONSTANT FOR WATER

$$Z_W = 1/HLC$$

5.3.3.1. Calculation of the Fugacity Capacity Constant, Z_W, for 4 - Chloro Biphenyl in terms of Experimental Input Data

$$HLC = 34.59 \text{ Pa m}^3\text{/mole}$$

$$Z_W = \frac{1}{HLC} = 2.89 \times 10^{-2} \text{ mole/m}^3\text{Pa}$$

5.3.3.2. Calculation of Fugacity Capacity Constant, Z_W, for 4 - Chloro Biphenyl in terms of Predicted Input Data

$$HLC = 35.96 \text{ Pa m}^3\text{/mole}$$

$$Z_W = \frac{1}{HLC} = 2.78 \times 10^{-2} \text{ mole/m}^3\text{Pa}$$

5.3.4. FUGACITY CAPACITY CONSTANT FOR BIOTA

$$Z_B = K_B \rho_B / HLC$$

$$\text{Log}K_B = \text{Log}K_{ow} - 1.32$$

5.3.4.1. Calculation of the Fugacity Capacity Constant, Z_B, for 4 - Chloro Biphenyl in terms of Experimental Data

$$\text{Log}\, K_B = 4.49 - 1.32$$

$$\text{Log}\, K_B = 3.17$$

$$K_B = 1479.10 \text{ m}^3\text{of water}/10^6\text{g biota}$$

$$\rho_B = 1 \times 10^6 \text{ g/m}^3$$

$$Z_B = 1479.10 \times 10^{-6} \times 1 \times 10^6 / 34.59$$

$$Z_B = 42.76 \text{ m}^3\text{/mole Pa}$$

5.3.4.2. Calculation of the Fugacity Capacity Constant, Z_B, for 4 - Chloro Biphenyl in terms of Predicted Input Data

$$\text{Log}\, K_B = 3.17$$

$$K_B = 1479.10 \text{ m}^3\text{of water}/10^6\text{g biota}$$

$$Z_B = 1479.10 \times 10^{-6} \times 1 \times 10^6 / 35.96$$

$$Z_B = 41.12 \text{ m}^3\text{/mole Pa}$$

5.3.5. FUGACITY CAPACITY CONSTANT FOR SEDIMENT AND SUSPENDED SOLIDS

$$Z_{sd} = K_{p\,sd} \times \rho_{sd} / HLC$$

$$Z_{ss} = K_{p\,ss} \times \rho_{ss} / HLC$$

5.3.5.1. Calculation of the Fugacity Capacity Constants, Z_{SD} and Z_{SS}, for 4- Chloro Biphenyl in terms of Experimental Data

$$K_{p\,sd} = \%OC \times K_{oc} \quad \text{m}^3\text{of water}/10^6\text{g sorbent}$$

$$K_{oc} = 2811.9$$

$$K_{p\,sd} = 0.04 \times 2811.9 \times 10^{-6} \text{ m}^3\text{of water/g sorbent}$$

$K_{p\,sd} = 112.5 \times 10^{-6}$

$\rho_{sd} = 1.5 \times 10^{6}$ g/m^3

$Z_{sd} = 112.5 \times 10^{-6} \times 1.5 \times 10^{6} / 34.59$

$Z_{sd} = 4.855$

For suspended solid and sediment % OC and density are the same. So, their fugacity capacity constants (Z_{ss}, Z_{sd}) have the same value.

$Z_{ss} = 4.855$

5.5.5.2. Calculation of Fugacity Capacity Constants, Z_{SD} and Z_{SS}, for 4 - Chloro Biphenyl in terms of Predicted Input Data

$K_{oc} = 2811.9$

$K_{p\,sd} = 112.5 \times 10^{-6}$ m^{3}of water/g sorbent

$Z_{sd} = 112.5 \times 10^{-6} \times 1.5 \times 10^{6} / 35.96$

$Z_{sd} = 4.669$

The fugacity capacity constants for air, soil, water, biota, suspended solids and sediment were computed for all congeners by using a BASIC program. The results are given in Appendix V. The results of the Specimen Calculation above are tabulated in Table 5.9. for comparison.

Table 5.9. Fugacity Capacity Constants Computed by Experimental and Predicted Input Data for 4 - Chloro Biphenyl.

	Z_A	Z_S	Z_W	Z_B	Z_{SS}&Z_{SD}
Calculated values with experimental input data	4.04×10^{-4}	2.43	2.89×10^{-2}	42.76	4.855
Calculated values with predicted input data	4.04×10^{-4}	2.33	2.78×10^{-2}	41.12	4.669

5.4. COMPUTATION OF COMPARTMENTAL DISTRIBUTION

The mass and equilibrium distributions, amount and concentrations of each congener were computed for each compartment using the same computer program which computed the fugacity capacity constants (Z_A, Z_W, Z_B, Z_S, Z_{SS}, Z_{SD}).

Mackay's Fugacity Model I assumes equilibrium between all phases. Equilibrium between all phases is defined as occurring when their fugacities are equal. It assumes that each compartment is well mixed and there is no reaction and advection into or out of the system. At equilibrium

$$f = f_A = f_W = f_S = f_B$$

where A, W, S, B represent the compartments.

A total amount M (mol) of chemical is introduced into the

system. If m_i (mol) and V_i (m^3) are the amounts and volumes for each compartment then the total amount M is given by

$$M = \sum m_i = \sum C_i V_i = \sum f_i Z_i V_i = f \sum Z_i V_i$$

$$f = \frac{M}{\sum V_i Z_i}$$

Since M is known f may be calculated. The amount in each compartment is given by:

$$m_i = f V_i Z_i$$

and the percentage by 100 m_i/M. The phase concentrations can be calculated from,

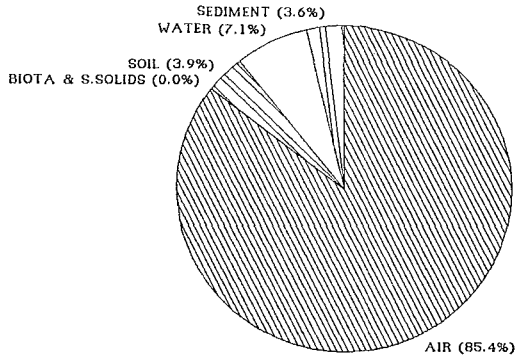
$$C_i = Z_i f$$

also equilibrium partitioning can be computed by:

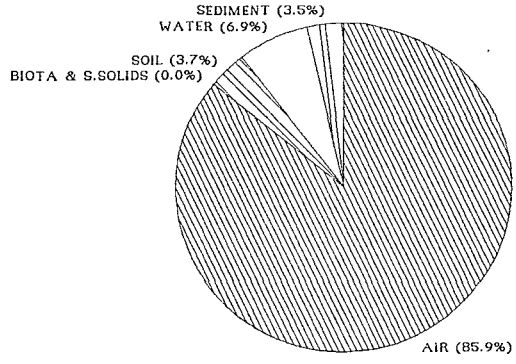
$$P_i' = \frac{Z_i}{\sum Z_i}$$

This Model provides information for each phase on (1) relative concentration (2)relative mass distributions. As an example, mass distribution (%) or amount (mole) and equilibrium distribution (%) results obtained by computing compartmentalization distribution of 4 - chloro biphenyl in each phase are given in the pie chart plot for experimental and predicted input data.

Mass Distribution[1] (%) of 4-Chloro Biphenyl



Mass Distribution[2] (%) of 4-Chloro Biphenyl



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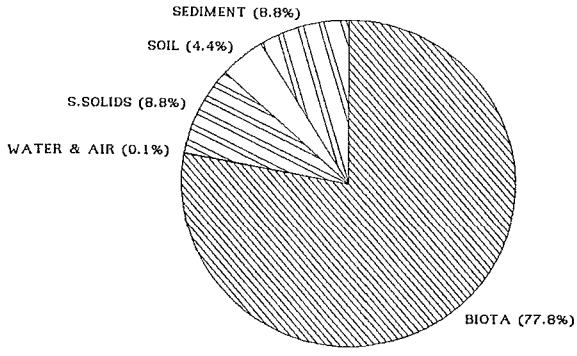
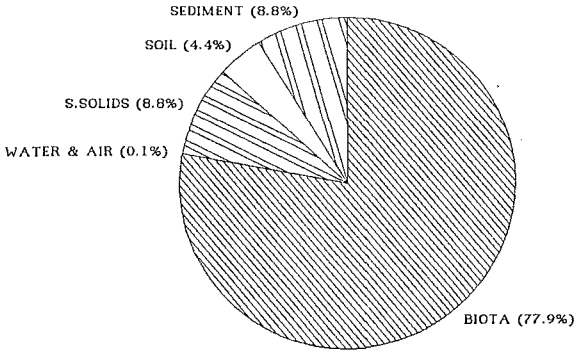
1 Calculated from Experimental Input Data

2 Calculated from Predicted Input Data
* % of Biota & S.Solids is less than 0.1

Equilibrium Distribution[3] (%) of 4-Chloro Biphenyl



Equilibrium Distribution[4] (%) of 4-Chloro Biphenyl



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3 Calculated from Experimental Input Data

4 Calculated from Predicted Input Data

VI. RESULTS AND DISCUSSION

6.1. THE CHARACTERISTIC ROOT INDEX AND PHYSICOCHEMICAL PROPERTIES.

This work shows that there exists an obvious relationship between physicochemical properties of PCBs and the CR index. It has been previously indicated that the CR index for describing the structure of a molecule has its roots in topology and comprises knowledge of size, heteroatom, and cyclization of structural graph and leads to values encoding considerable structural information such as total surface area which was discussed in section V. The logarithm of water solubility, vapour pressure and octanol-water partition coefficient were regressed against the CR index by the method of least squares and regression analysis were performed with Lotus 123 package. The results of regression analyses for water solubility, vapour pressure and octanol-water partition coefficient are also given in section V. Comparison of the observed and predicted physicochemical properties clearly demonstrates that the CR index is very accurate in predicting the physicochemical properties.

It is important to realize that the coefficients obtained in regressions are applicable only to PCB's. It is also noted that other chemicals can be included in the regression analysis, if one wishes to estimate their physicochemical properties. Thus the range of applicability of the CR index model can be extended to the other pollutants which are important from the environmental point of view, such as alkyl benzenes, heterocyclic PAHs, substituted PAHs, and chlorophenols etc.

On the other hand each congener is characterized by a single number without rounding off the numbers up to four digits after the decimal point. The corresponding zero and first order molecular connectivity index which is most widely used in QSAR studies can not characterize members of the same weight class of PCBs individually.

Finally CR index values can be easily obtained by using computer algorithms, and a complete tabulation for all PCB congeners and for other chemicals is also possible.

6.2. TABULATION OF THE RESULTS

The results of the compartmental distribution of PCB congeners are given in Table 6 where, calculated$^{(a)}$ represents the calculated distribution according to the experimental input data (water solubility, vapour pressure and octanol water partition coefficient) and calculated$^{(b)}$ represents the calculated distribution according to the predicted input data. Among the PCB congeners, only 21 have a complete set of experimental physicochemical properties. One of the input data either vapour pressure, solubility or octanol-water partition

coefficient is missing for about 10 congeners. Although they appear in the single correlation their experimental values can not be included in Model I calculations because of the lack of one of the input data. So, the compartmental distribution of 21 PCB congeners was calculated with both experimental and predicted input data. However, the compartmental distribution of the remaining 37 PCBs was calculated with only predicted input data.

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

AIR				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	91.36	91.08	3.25E-03	3.22E-03
2-chloro	92.32	86.68	1.87E-04	9.01E-04
4-	85.39	85.87	7.34E-04	7.64E-04
2-2'-dichloro	80.29	77.62	2.59E-04	2.22E-04
4-4'-	84.80	75.97	3.96E-04	1.84E-04
2-5-	67.34	76.44	1.16E-04	1.94E-04
2-6-	-	76.88	-	2.04E-04
2-4'-	86.20	76.96	3.45E-04	2.06E-04
3-3'-	-	76.44	-	1.96E-04
3-4-	-	77.09	-	2.09E-04
2-2'-4-trichloro	-	61.18	-	5.04E-05
2-2'-3-	-	60.66	-	4.85E-05
2-2'-5-	88.80	60.44	2.64E-04	4.77E-05
2-3-4'-	-	60.03	-	4.63E-05
2-4'-5-	-	61.26	-	5.07E-05
2-3-3'-	-	61.47	-	5.16E-05
3-4-4'-	-	62.96	-	5.77E-05
2-4-4'-	-	62.78	-	5.96E-05
2-4-5-	62.26	61.28	5.76E-05	5.08E-05
2-4-6-	62.37	60.80	5.34E-05	4.90E-05
2-2'-3-4-tetra	-	40.96	-	1.24E-05
2-2'-3-3'-	-	41.29	-	1.27E-05
2-2'-3-5'-	-	39.19	-	1.11E-05
2-2'-4-4'-	56.67	38.71	2.48E-05	1.10E-05
2-3-4-4'-	-	45.32	-	1.67E-05
2-3'-4-4'-	-	40.16	-	1.18E-05
2-2'-5-5'-	42.24	37.98	1.19E-05	1.01E-05

Table 6. Continued

AIR				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	27.71	38.71	6.44E-06	1.06E-05
3-3'-4-4'-	20.85	40.40	4.51E-06	1.20E-05
2-3-5-6-	-	50.92	-	2.44E-05
2-4-4'-5-	-	41.17	-	1.27E-05
2-3-4-5-	-	44.17	-	1.55E-05
2-2'-5-6'-	-	38.68	-	1.07E-05
2-2'-4-5-	-	39.30	-	1.11E-05
2-2'-6-6'	-	41.08	-	1.25E-05
2-3'-4-4'-5-penta	-	22.39	-	3.00E-06
2-3-4-5-6-	-	25.64	-	4.00E-06
2-2'-3-4-4'-	-	22.66	-	3.08E-06
2-2'-3-5'-6-	-	21.12	-	2.67E-06
2-2'-3-4-5'-	39.32	21.64	2.81E-06	5.99E-06
2-2'-3'-4-5-	-	23.14	-	3.22E-06
2-2'-4-4'-5-	-	21.92	-	2.87E-06
2-2'-4-6-6'-	-	21.74	-	2.83E-06
2-2'-4-5-5'-	13.91	26.65	1.49E-06	2.55E-06
2-3-3'-4'-6-	-	23.11	-	3.21E-06
2-3-3'-4-4'-	-	22.93	-	3.16E-06
2-2'-3-3'-6-6'-hexa	1.33	10.59	1.29E-07	7.36E-07
2-2'-3-4-4'-5-	-	12.05	-	9.27E-07
2-2'-3-4-5-5'-	-	10.56	-	7.32E-07
2-2'-3-4'-5-5'-	-	10.75	-	7.56E-07
2-2'-4-4'-5-5'-	14.26	10.65	8.87E-07	7.44E-07
2-2'-3-3'-4-4'-	22.18	12.19	2.37E-06	9.46E-07
2-2'-4-4'-6-6'-	31.69	8.43	2.23E-06	4.96E-07
2-2'-4-5-5'-6-	-	9.74	-	6.37E-07
2-2'-3-3'-4-4'-6-	-	4.87	-	1.99E-07
2-2'-3-3'-4-4'-5-5'-	-	2.11	-	5.25E-08
2-2'-3-3'-4-5'-6-6'-	-	1.80	-	4.11E-08
2-2'-3-3'-5-5'-6-6'-	2.71	1.81	6.13E-08	4.15E-08

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

WATER				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	5.92	6.15	7.10E-02	1.80E-01
2-chloro	4.14	6.82	7.19E-02	6.07E-02
4-	7.13	6.90	5.26E-02	5.26E-02
2-2'-dichloro	6.29	7.17	1.73E-02	1.75E-02
4-4'-	5.26	7.15	2.11E-02	1.48E-02
2-5-	9.51	7.16	1.41E-02	1.55E-02
2-6-	-	7.17	-	1.62E-02
2-4'-	3.94	7.18	1.35E-02	1.64E-02
3-3'-	-	7.22	-	1.59E-02
3-4-	-	7.17	-	1.66E-02
2-2'-4-trichloro	-	6.66	-	4.70E-03
2-2'-3-	-	6.63	-	4.55E-03
2-2'-5-	2.00	6.62	5.09E-03	4.49E-03
2-3-4'-	-	6.59	-	4.36E-03
2-4'-5-	-	6.67	-	4.73E-03
2-3-3'-	-	6.69	-	4.82E-03
3-4-4'-	-	6.76	-	5.31E-03
2-4-4'-	-	6.75	-	5.25E-03
2-4-5-	-	6.67	-	4.74E-03
2-4-6-	6.50	6.65	4.78E-03	4.60E-03
2-2'-3-4-tetra	-	5.19	-	1.35E-03
2-2'-3-3'-	-	5.22	-	1.38E-03
2-2'-3-5'-	-	5.04	-	1.22E-03
2-2'-4-4'-	4.07	5.19	1.52E-03	1.26E-03
2-3-4-4'-	-	5.57	-	1.77E-03
2-2'-5-5'-	4.49	4.92	1.08E-03	1.13E-03
2-3'-4-4'-	-	5.12	-	1.29E-03

Table 6. Continued

WATER				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	5.84	4.99	1.16E-03	1.18E-03
3-3'-4-4'-	6.56	5.15	1.22E-03	1.31E-03
2-3-5-6-	-	6.01	-	2.47E-03
2-4-4'-5-	-	5.22	-	1.37E-03
2-3-4-5-	-	5.47	-	1.64E-03
2-2'-5-6'-	-	4.99	-	1.18E-03
2-2'-4-5-	-	5.05	-	1.22E-03
2-2'-6-6'	-	5.20	-	1.36E-03
2-3'-4-4'-5-penta	-	3.31	-	3.81E-04
2-3-4-5-6-	-	3.68	-	4.92E-04
2-2'-3-4-4'-	-	3.35	-	3.91E-04
2-2'-3-5'-6-	-	3.16	-	3.43E-04
2-2'-3-4-5'-	2.19	3.23	2.86E-04	3.59E-04
2-2'-3'-4-5-	-	3.40	-	4.06E-04
2-2'-4-4'-5-	-	3.25	-	3.66E-04
2-2'-4-6-6'-	-	3.23	-	3.61E-04
2-2'-4-5-5'-	3.10	3.11	2.86E-04	3.29E-04
2-3-3'-4'-6-	-	3.39	-	4.04E-04
2-3-3'-4-4'-	-	3.37	-	3.89E-04
2-2'-3-3'-6-6'-hexa	3.75	1.82	3.13E-04	1.08E-04
2-2'-3-4-4'-5-	-	2.02	-	1.33E-04
2-2'-3-4-5-5'-	-	1.81	-	1.08E-04
2-2'-3-4'-5-5'-	-	1.84	-	1.13E-04
2-2'-4-4'-5-5'-	1.39	1.83	7.45E-05	1.09E-04
2-2'-3-3'-4-4'-	2.42	2.04	2.22E-04	1.36E-04
2-2'-4-4'-6-6'-	0.95	1.51	5.79E-05	7.64E-05
2-2'-4-5-5'-6-	-	1.70	-	9.55E-05
2-2'-3-3'-4-4'-6-	-	0.97	-	3.39E-05
2-2'-3-3'-4-4'-5-5'-	-	0.48	-	1.02E-05
2-2'-3-3'-4-5'-6-6'-	-	0.42	-	8.27E-06
2-2'-3-3'-5-5'-6-6'-	-	0.45	-	8.35E-06

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

	AIR		WATER	
	CONCENTRATION (ppm)		CONCENTRATION (ppm)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	1.97E-03	1.96E-03	1.30E-04	1.35E-04
2-chloro	2.44E-03	2.29E-03	1.83E-04	1.11E-04
4-	2.26E-03	2.27E-03	1.92E-04	1.86E-04
2-2'-dichloro	2.50E-03	2.42E-03	2.00E-04	2.87E-04
4-4'-	2.65E-03	2.37E-03	1.67E-04	2.28E-04
2-5-	2.10E-03	2.38E-03	3.03E-04	2.28E-04
2-6-	-	2.40E-03	-	2.29E-04
2-4'-	2.69E-03	2.40E-03	1.25E-04	2.29E-04
3-3'-	-	2.39E-03	-	2.30E-04
3-4-	-	2.41E-03	-	2.29E-04
2-2'-4-trichloro	-	2.20E-03	-	2.45E-04
2-2'-3-	-	2.19E-03	-	2.44E-04
2-2'-5-	2.18E-03	3.20E-03	7.36E-05	2.43E-04
2-3-4'-	-	2.16E-03	-	2.42E-04
2-4'-5-	-	2.20E-03	-	2.45E-04
2-3-3'-	-	2.21E-03	-	2.46E-04
3-4-4'-	-	2.27E-03	-	2.48E-04
2-4-4'-	-	2.26E-03	-	2.48E-04
2-4-5-	2.26E-03	2.21E-03	-	2.45E-04
2-4-6-	2.24E-03	2.19E-03	2.39E-04	2.44E-04
2-2'-3-4-tetra	-	1.67E-03	-	2.17E-04
2-2'-3-3'-	-	1.68E-03	-	2.17E-04
2-2'-3-5'-	-	1.60E-03	-	2.11E-04
2-2'-4-4'-	2.31E-03	1.58E-03	1.70E-04	2.16E-04
2-3-4-4'-	-	1.85E-03	-	2.32E-04
2-2'-5-5'-	1.72E-03	1.55E-03	1.87E-04	2.05E-04
2-3'-4-4'-	-	1.64E-03	-	2.14E-04

Table 6. Continued

	AIR		WATER	
	CONCENTRATION (ppm)		CONCENTRATION (ppm)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	1.13E-03	1.58E-03	2.43E-04	2.08E-04
3-3'-4-4'-	8.52E-04	1.65E-03	2.73E-04	2.15E-04
2-3-5-6-	-	2.08E-03	-	2.50E-04
2-4-4'-5-	-	1.68E-03	-	2.17E-04
2-3-4-5-	-	1.81E-03	-	2.28E-04
2-2'-5-6'-	-	1.58E-03	-	2.08E-04
2-2'-4-5-	-	1.61E-03	-	2.11E-04
2-2'-6-6'	-	1.68E-03	-	2.17E-04
2-3'-4-4'-5-penta	-	1.02E-03	-	1.54E-04
2-3-4-5-6-	-	1.17E-03	-	1.72E-04
2-2'-3-4-4'-	-	1.03E-03	-	1.56E-04
2-2'-3-5'-6-	-	9.65E-04	-	1.47E-04
2-2'-3-4-5'-	1.77E-03	9.89E-04	1.02E-04	1.02E-04
2-2'-3'-4-5-	-	1.06E-03	-	1.58E-04
2-2'-4-4'-5-	-	1.00E-03	-	1.51E-04
2-2'-4-6-6'-	-	9.94E-04	-	1.51E-04
2-2'-4-5-5'-	6.36E-04	9.44E-04	1.44E-04	1.45E-04
2-3-3'-4'-6-	-	1.06E-03	-	1.58E-04
2-3-3'-4-4'-	-	1.05E-03	-	1.57E-04
2-2'-3-3'-6-6'-hexa	6.72E-05	5.35E-04	1.93E-04	9.40E-05
2-2'-3-4-4'-5-	-	6.09E-04	-	1.04E-04
2-2'-3-4-5-5'-	-	5.34E-04	-	9.37E-05
2-2'-3-4'-5-5'-	-	5.43E-04	-	9.52E-05
2-2'-4-4'-5-5'-	7.20E-04	5.38E-04	7.20E-05	9.45E-05
2-2'-3-3'-4-4'-	1.12E-03	6.16E-04	1.25E-04	1.05E-04
2-2'-4-4'-6-6'-	1.60E-03	4.26E-04	4.93E-05	7.80E-05
2-2'-4-5-5'-6-	-	4.92E-04	-	8.79E-05
2-2'-3-3'-4-4'-6-	-	2.69E-04	-	5.45E-05
2-2'-3-3'-4-4'-5-5'-	-	1.26E-04	-	2.95E-05
2-2'-3-3'-4-5'-6-6'-	-	1.08E-04	-	2.59E-05
2-2'-3-3'-5-5'-6-6'-	1.63E-04	1.09E-04	-	2.61E-05

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

SOIL				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	1.40	1.42	6.64	6.71
2-chloro	1.82	3.53	4.92	4.64
4-	3.85	3.72	4.41	4.41
2-2'-dichloro	6.91	7.83	2.97	2.98
4-4'-	5.11	8.69	3.19	2.80
2-5-	11.92	8.44	2.75	2.85
2-6-	-	8.21	-	2.90
2-4'-	5.07	8.17	2.70	2.90
3-3'-	-	8.39	-	2.87
3-4-	-	8.11	-	2.92
2-2'-4-trichloro	-	16.55	-	1.81
2-2'-3-	-	16.83	-	1.79
2-2'-5-	4.73	16.94	1.87	1.78
2-3-4'-	-	17.17	-	1.76
2-4'-5-	-	16.50	-	1.82
2-3-3'-	-	16.38	-	1.83
3-4-4'-	-	15.58	-	1.90
2-4-4'-	-	15.68	-	1.89
2-4-5-	15.66	16.49	1.92	1.82
2-4-6-	16.02	16.75	1.82	1.80
2-2'-3-4-tetra	-	27.63	-	1.12
2-2'-3-3'-	-	27.45	-	1.13
2-2'-3-5'-	-	28.61	-	1.07
2-2'-4-4'-	20.15	28.78	1.17	1.09
2-3-4-4'-	-	25.22	-	1.24
2-2'-5-5'-	27.32	29.29	1.03	1.04
2-3'-4-4'-	-	28.08	-	1.01

Table 6. Continued

SOIL				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	34.09	28.88	1.06	1.06
3-3'-4-4'-	37.25	27.94	1.07	1.11
2-3-5-6-	-	22.14	-	1.41
2-4-4'-5-	-	27.51	-	1.12
2-3-4-5-	-	25.85	-	1.21
2-2'-5-6'-	-	28.89	-	1.06
2-2'-4-5-	-	28.55	-	1.07
2-2'-6-6'	-	27.56	-	1.12
2-3'-4-4'-5-penta	-	37.96	-	0.679
2-3-4-5-6-	-	36.15	-	0.752
2-2'-3-4-4'-	-	37.80	-	0.686
2-2'-3-5'-6-	-	38.66	-	0.651
2-2'-3-4-5'-	29.84	38.37	0.606	0.663
2-2'-3'-4-5-	-	37.54	-	0.697
2-2'-4-4'-5-	-	38.22	-	0.669
2-2'-4-6-6'-	-	38.32	-	0.665
2-2'-4-5-5'-	42.33	38.92	0.606	0.641
2-3-3'-4'-6-	-	37.56	-	0.695
2-3-3'-4-4'-	-	37.66	-	0.691
2-2'-3-3'-6-6'-hexa	48.45	44.41	0.628	0.411
2-2'-3-4-4'-5-	-	43.63	-	0.447
2-2'-3-4-5-5'-	-	44.43	-	0.410
2-2'-3-4'-5-5'-	-	44.32	-	0.415
2-2'-4-4'-5-5'-	42.63	44.38	0.353	0.413
2-2'-3-3'-4-4'-	38.41	43.56	0.548	0.450
2-2'-4-4'-6-6'-	-	45.53	-	0.357
2-2'-4-5-5'-6-	-	44.85	-	0.390
2-2'-3-3'-4-4'-6-	-	47.20	-	0.257
2-2'-3-3'-4-4'-5-5'-	-	47.94	-	0.159
2-2'-3-3'-4-5'-6-6'-	-	47.91	-	0.145
2-2'-3-3'-5-5'-6-6'-	47.42	47.92	0.143	0.146

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

BIOTA				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION(%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	2.18E-03	2.18E-03	66.57	66.23
2-chloro	4.33E-03	8.60E-03	75.32	76.71
4-	1.05E-02	1.02E-02	77.84	77.84
2-2'-dichloro	3.08E-02	3.47E-02	85.12	85.06
4-4'-	2.09E-02	4.15E-02	84.02	85.96
2-5-	5.81E-02	3.94E-02	86.22	85.71
2-6-	-	3.76E-02	-	85.47
2-4'-	2.52E-02	3.72E-02	86.44	85.41
3-3'-	-	3.88E-02	-	85.60
3-4-	-	3.68E-02	-	85.35
2-2'-4-trichloro	-	0.128	-	90.90
2-2'-3-	-	0.132	-	91.01
2-2'-5-	0.036	0.134	90.62	91.06
2-3-4'-	-	0.137	-	91.16
2-4'-5-	-	0.128	-	90.88
2-3-3'-	-	0.126	-	90.81
3-4-4'-	-	0.115	-	90.46
2-4-4'-	-	0.116	-	90.50
2-4-5-	0.114	0.127	90.38	90.87
2-4-6-	0.123	0.131	90.85	90.98
2-2'-3-4-tetra	-	0.361	-	94.39
2-2'-3-3'-	-	0.356	-	94.34
2-2'-3-5'-	-	0.391	-	94.61
2-2'-4-4'-	0.250	0.387	94.11	94.53
2-3-4-4'-	-	0.295	-	93.77
2-2'-5-5'-	0.391	0.413	94.85	94.77
2-3'-4-4'-	-	0.374	-	94.49

Table 6. Continued

BIOTA				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION(%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	0.475	0.399	94.71	94.68
3-3'-4-4'-	0.509	0.370	94.61	94.45
2-3-5-6-	-	0.225	-	92.89
2-4-4'-5-	-	0.357	-	94.35
2-3-4-5-	-	0.312	-	93.94
2-2'-5-6'-	-	0.400	-	94.68
2-2'-4-5-	-	0.389	-	94.60
2-2'-6-6'	-	0.359	-	94.37
2-3'-4-4'-5-penta	-	0.839	-	96.60
2-3-4-5-6-	-	0.719	-	96.23
2-2'-3-4-4'-	-	0.826	-	96.56
2-2'-3-5'-6-	-	0.892	-	96.74
2-2'-3-4-5'-	0.742	0.869	96.96	96.68
2-2'-3'-4-5-	-	0.808	-	96.51
2-2'-4-4'-5-	-	0.858	-	96.65
2-2'-4-6-6'-	-	0.865	-	96.67
2-2'-4-5-5'-	1.050	0.914	96.96	96.79
2-3-3'-4'-6-	-	0.810	-	96.52
2-3-3'-4-4'-	-	0.817	-	96.54
2-2'-3-3'-6-6'-hexa	1.160	1.644	96.85	97.94
2-2'-3-4-4'-5-	-	1.483	-	97.76
2-2'-3-4-5-5'-	-	1.647	-	97.94
2-2'-3-4'-5-5'-	-	1.624	-	97.92
2-2'-4-4'-5-5'-	1.840	1.635	98.23	97.93
2-2'-3-3'-4-4'-	1.050	1.469	97.25	97.74
2-2'-4-4'-6-6'-	1.625	1.946	98.40	98.21
2-2'-4-5-5'-6-	-	1.749	-	98.04
2-2'-3-3'-4-4'-6-	-	2.812	-	98.71
2-2'-3-3'-4-4'-5-5'-	-	4.640	-	99.20
2-2'-3-3'-4-5'-6-6'-	-	5.07	-	99.27
2-2'-3-3'-5-5'-6-6'-	5.12	5.05	99.28	99.26

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

	SOIL		BIOTA	
	CONCENTRATION (ppm)		CONCENTRATION (ppm)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	3.19E-03	3.25E-03	0.05	0.05
2-chloro	5.09E-03	9.37E-03	0.12	0.23
4-	1.08E-02	1.04E-02	0.28	0.28
2-2'-dichloro	2.28E-02	2.59E-02	0.98	1.11
4-4'-	1.69E-02	2.87E-02	0.67	1.32
2-5-	3.94E-02	2.79E-02	1.85	1.26
2-6-	-	2.71E-02	-	1.20
2-4'-	1.67E-02	2.70E-02	0.80	1.19
3-3'-	-	2.77E-02	-	1.24
3-4-	-	2.68E-02	-	1.17
2-2'-4-trichloro	-	6.31E-02	-	4.74
2-2'-3-	-	6.42E-02	-	4.88
2-2'-5-	1.81E-02	6.46E-02	1.31	4.94
2-3-4'-	-	6.55E-02	-	5.07
2-4'-5-	-	6.29E-02	-	4.71
2-3-3'-	-	6.25E-02	-	4.64
3-4-4'-	-	5.94E-02	-	4.23
2-4-4'-	-	5.98E-02	-	4.28
2-4-5-	5.97E-02	6.29E-02	4.21	4.70
2-4-6-	6.11E-02	6.39E-02	4.55	4.84
2-2'-3-4-tetra	-	0.110	-	15.09
2-2'-3-3'-	-	0.118	-	14.86
2-2'-3-5'-	-	0.123	-	16.31
2-2'-4-4'-	0.087	0.124	10.46	16.15
2-3-4-4'-	-	0.109	-	12.32
2-2'-5-5'-	0.118	0.126	16.33	17.25
2-3'-4-4'-	-	0.121	-	15.64

Table 6. Continued

	SOIL		BIOTA	
	CONCENTRATION (ppm)		CONCENTRATION (ppm)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	0.147	0.124	19.82	16.68
3-3'-4-4'-	0.161	0.120	21.25	15.44
2-3-5-6-	-	0.095	-	9.40
2-4-4'-5-	-	0.119	-	14.92
2-3-4-5-	-	0.111	-	13.01
2-2'-5-6'-	-	0.125	-	16.71
2-2'-4-5-	-	0.123	-	16.24
2-2'-6-6'	-	0.119	-	14.99
2-3'-4-4'-5-penta	-	0.183	-	39.15
2-3-4-5-6-	-	0.174	-	33.54
2-2'-3-4-4'-	-	0.182	-	38.55
2-2'-3-5'-6-	-	0.186	-	41.62
2-2'-3-4-5'-	0.144	0.185	34.62	40.55
2-2'-3'-4-5-	-	0.181	-	37.68
2-2'-4-4'-5-	-	0.184	-	40.04
2-2'-4-6-6'-	-	0.185	-	40.37
2-2'-4-5-5'-	-	0.188	49.11	42.62
2-3-3'-4'-6-	-	0.181	-	37.80
2-3-3'-4-4'-	-	0.182	-	38.11
2-2'-3-3'-6-6'-hexa	0.259	0.237	59.87	84.77
2-2'-3-4-4'-5-	-	0.233	-	76.48
2-2'-3-4-5-5'-	-	0.237	-	84.95
2-2'-3-4'-5-5'-	-	0.237	-	83.73
2-2'-4-4'-5-5'-	0.227	0.237	94.94	84.31
2-2'-3-3'-4-4'-	0.205	0.232	54.61	75.78
2-2'-4-4'-6-6'-	-	0.243	83.82	100.35
2-2'-4-5-5'-6-	-	0.239	-	90.21
2-2'-3-3'-4-4'-6-	-	0.276	-	158.82
2-2'-3-3'-4-4'-5-5'-	-	0.305	-	285.15
2-2'-3-3'-4-5'-6-6'-	-	0.305	-	311.43
2-2'-3-3'-5-5'-6-6'-	0.305	0.301	314.38	310.29

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

SUSPENDED SOLIDS				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	2.17E-03	2.21E-03	13.29	13.42
2-chloro	2.83E-03	5.21E-03	9.84	9.29
4-	5.99E-03	5.79E-03	8.83	8.83
2-2'-dichloro	1.07E-02	1.21E-02	5.94	5.96
4-4'-	7.96E-03	1.35E-02	6.38	5.60
2-5-	1.85E-02	1.31E-02	5.50	5.70
2-6-	-	1.27E-02	-	5.80
2-4'-	7.89E-03	1.27E-02	5.41	5.82
3-3'-	-	1.31E-02	-	5.75
3-4-	-	1.26E-02	-	5.85
2-2'-4-trichloro	-	2.57E-02	-	3.63
2-2'-3-	-	2.61E-02	-	3.59
2-2'-5-	7.36E-03	2.63E-02	3.74	3.57
2-3-4'-	-	2.67E-02	-	3.53
2-4'-5-	-	2.56E-02	-	3.64
2-3-3'-	-	2.54E-02	-	3.67
3-4-4'-	-	2.42E-02	-	3.81
2-4-4'-	-	2.43E-02	-	3.79
2-4-5-	2.44E-02	2.56E-02	3.84	3.64
2-4-6-	2.49E-02	2.60E-02	3.65	3.60
2-2'-3-4-tetra	-	4.29E-02	-	2.24
2-2'-3-3'-	-	4.27E-02	-	2.26
2-2'-3-5'-	-	4.45E-02	-	2.15
2-2'-4-4'-	3.13E-02	4.47E-02	2.35	2.18
2-3-4-4'-	-	3.92E-02	-	2.49
2-2'-5-5'-	4.25E-02	4.55E-02	2.05	2.08
2-3'-4-4'-	-	4.36E-02	-	2.20

Table 6. Continued

SUSPENDED SOLIDS				
	MASS DISTRIBUTION (%)		EQUILIBRIUM DISTRIBUTION (%)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	5.30E-02	4.49E-02	2.11	2.12
3-3'-4-4'-	5.79E-02	4.34E-02	2.15	2.21
2-3-5-6-	-	3.44E-02	-	2.83
2-4-4'-5-	-	4.28E-02	-	2.25
2-3-4-5-	-	4.02E-02	-	2.42
2-2'-5-6'-	-	4.49E-02	-	2.12
2-2'-4-5-	-	4.44E-02	-	2.16
2-2'-6-6'	-	4.28E-02	-	2.25
2-3'-4-4'-5-penta	-	5.90E-02	-	1.36
2-3-4-5-6-	-	5.62E-02	-	1.50
2-2'-3-4-4'-	4.64E-02	5.88E-02	1.21	1.37
2-2'-3-5'-6-	-	6.01E-02	-	1.30
2-2'-3-4-5'-	-	5.96E-02	-	1.32
2-2'-3'-4-5-	-	5.83E-02	-	1.39
2-2'-4-4'-5-	-	5.94E-02	-	1.34
2-2'-4-6-6'-	-	5.96E-02	-	1.33
2-2'-4-5-5'-	6.58E-02	6.05E-02	1.21	1.28
2-3-3'-4'-6-	-	5.84E-02	-	1.39
2-3-3'-4-4'-	-	5.85E-02	-	1.38
2-2'-3-3'-6-6'-hexa	7.53E-02	6.90E-02	1.25E+00	8.20E-02
2-2'-3-4-4'-5-	-	6.78E-02	-	8.90E-02
2-2'-3-4-5-5'-	-	6.91E-02	-	8.20E-02
2-2'-3-4'-5-5'-	-	6.89E-02	-	8.30E-02
2-2'-4-4'-5-5'-	6.63E-02	6.90E-02	7.07E-01	8.26E-02
2-2'-3-3'-4-4'-	5.97E-02	6.77E-02	1.09E+00	9.01E-02
2-2'-4-4'-6-6'-	5.28E-02	7.08E-02	6.39E-01	7.14E-02
2-2'-4-5-5'-6-	-	6.90E-02	-	7.81E-02
2-2'-3-3'-4-4'-6-	-	7.34E-02	-	5.15E-03
2-2'-3-3'-4-4'-5-5'-	-	7.45E-02	-	3.18E-02
2-2'-3-3'-4-5'-6-6'-	-	7.45E-02	-	2.90E-02
2-2'-3-3'-5-5'-6-6'-	7.37E-02	7.45E-02	2.86E-01	2.92E-02

Table 6. Results of Compartmental Distribution Values for PCB Congeners Computed by Experimental[a] and Predicted[b] Input Data, Using Mackay Fugacity Model I.

SEDIMENT				
	MASS DISTRIBUTION (%)		CONCENTRATION (ppm)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
Biphenyl	1.31	1.32	6.39E-03	6.50E-03
2-chloro	1.70	3.12	1.01E-02	1.87E-02
4-	3.59	3.47	2.15E-02	2.08E-02
2-2'-dichloro	6.45	7.31	4.57E-02	5.18E-02
4-4'-	4.77	8.11	3.38E-02	5.74E-02
2-5-	11.13	7.88	7.88E-02	5.58E-02
2-6-	-	7.67	-	5.43E-02
2-4'-	4.73	7.67	3.35E-02	5.40E-02
3-3'-	-	7.83	-	5.55E-02
3-4-	-	7.57	-	5.36E-02
2-2'-4-trichloro	-	15.44	-	0.126
2-2'-3-	-	15.70	-	0.128
2-2'-5-	4.41	15.81	0.036	0.129
2-3-4'-	-	16.02	-	0.131
2-4'-5-	-	15.40	-	0.125
2-3-3'-	-	15.29	-	0.125
3-4-4'-	-	14.54	-	0.118
2-4-4'-	-	14.63	-	0.119
2-4-5-	14.62	15.39	0.119	0.125
2-4-6-	14.95	15.63	0.025	0.127
2-2'-3-4-tetra	-	25.79	-	0.239
2-2'-3-3'-	-	25.62	-	0.237
2-2'-3-5'-	-	26.70	-	0.247
2-2'-4-4'-	18.81	26.86	0.174	0.249
2-3-4-4'-	-	23.53	-	0.218
2-2'-5-5'-	25.50	27.34	0.236	0.253
2-3'-4-4'-	-	26.20	-	0.242

Table 6. Continued

SEDIMENT				
	MASS DISTRIBUTION (%)		CONCENTRATION (ppm)	
CONGENER NO	Calc.[a]	Calc.[b]	Calc.[a]	Calc.[b]
2-3'-4'-5-	31.81	26.95	0.294	0.249
3-3'-4-4'-	34.76	26.07	0.322	0.241
2-3-5-6-	-	20.66	-	0.191
2-4-4'-5-	-	25.68	-	0.238
2-3-4-5-	-	24.13	-	0.223
2-2'-5-6'-	-	26.97	-	0.250
2-2'-4-5-	-	26.65	-	0.247
2-2'-6-6'	-	25.73	-	0.238
2-3'-4-4'-5-penta	-	35.43	-	0.367
2-3-4-5-6-	-	33.74	-	0.349
2-2'-3-4-4'-	-	35.28	0.288	0.365
2-2'-3-5'-6-	-	36.09	-	0.373
2-2'-3-4-5'-	27.85	35.81	-	0.371
2-2'-3'-4-5-	-	35.03	-	0.363
2-2'-4-4'-5-	-	35.67	-	0.369
2-2'-4-6-6'-	-	35.76	-	0.370
2-2'-4-5-5'-	39.51	36.33	0.409	0.376
2-3-3'-4'-6-	-	35.05	-	0.363
2-3-3'-4-4'-	-	35.15	-	0.364
2-2'-3-3'-6-6'-hexa	45.22	41.45	0.518	0.474
2-2'-3-4-4'-5-	-	40.72	-	0.466
2-2'-3-4-5-5'-	-	41.46	-	0.475
2-2'-3-4'-5-5'-	-	41.37	-	0.474
2-2'-4-4'-5-5'-	39.79	41.42	0.455	0.474
2-2'-3-3'-4-4'-	35.85	40.65	0.410	0.465
2-2'-4-4'-6-6'-	31.70	42.49	0.363	0.486
2-2'-4-5-5'-6-	-	41.86	-	0.479
2-2'-3-3'-4-4'-6-	-	44.06	-	0.055
2-2'-3-3'-4-4'-5-5'-	-	44.74	-	0.610
2-2'-3-3'-4-5'-6-6'-	-	44.71	-	0.610
2-2'-3-3'-5-5'-6-6'-	44.26	44.71	0.603	0.610

6.3. EVALUATION OF MODEL RESULTS

The Level I Model converts the physical data to fugacity capacities, Z_i, and calculates partitioning behaviour of the chemical in the evaluative environment. The absolute concentrations of the compounds predicted to be in various compartments 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 Table 4.1).

There is a high correlation between the calculated results with both types of input data and the relations are of the form $y = mx$, where the intercept is exactly zero. However, there is a discrepancy in mass distribution and concentration values of both air and water compartments. The discrepancy arises because the model predicts the equilibrium distributions based on thermodynamic criteria, without taking into account the kinetics of water exchange process, which limit atmospheric concentration. On the other hand, the fugacity capacity constant for air does not depend on the physical or chemical properties of the molecule. It only depends on the temperature and universal gas constant. So, the resulting poor relations between the calculated values of both mass distribution and concentration in the air compartment can not arise from the predicted input data. In the water compartment, the fugacity capacity constant depends only on Henry's Law Constant. Therefore, the contrasts both in mass distribution and concentration values in the water compartment arise from the discrepancies between the calculated values of HLCs, discussed in section V.

In accordance with the previously proposed procedure, mass and equilibrium distributions and concentrations of PCBs in various compartments of the environment were calculated with experimental and predicted input data. These are given in Fig.6.1. through Fig. 6.3. We can say that this model predicts reasonable equilibrium distribution for all compartments, mass distribution and concentration for the compartments other than air and water.

Mass distribution values give information on where most of the quantity of chemical may partition, and equilibrium distribution values reflect where the highest concentrations may occur at equilibrium. Both forms are therefore of use in assessments. For instance, the percentage of a chemical in biota is generally negligible from the point of view of mass balance, but it is significant when considered as a relative concentration. The more chlorinated PCB forms seem to be more soluble in lipids, and they are accumulated in biota rather than the less chlorinated forms. PCBs reach high concentrations in biota, thus that is where PCBs partition mostly in the environment, after equilibrium has been reached. From the partitioning patterns it is easy to visualize the areas that need to be further studied.

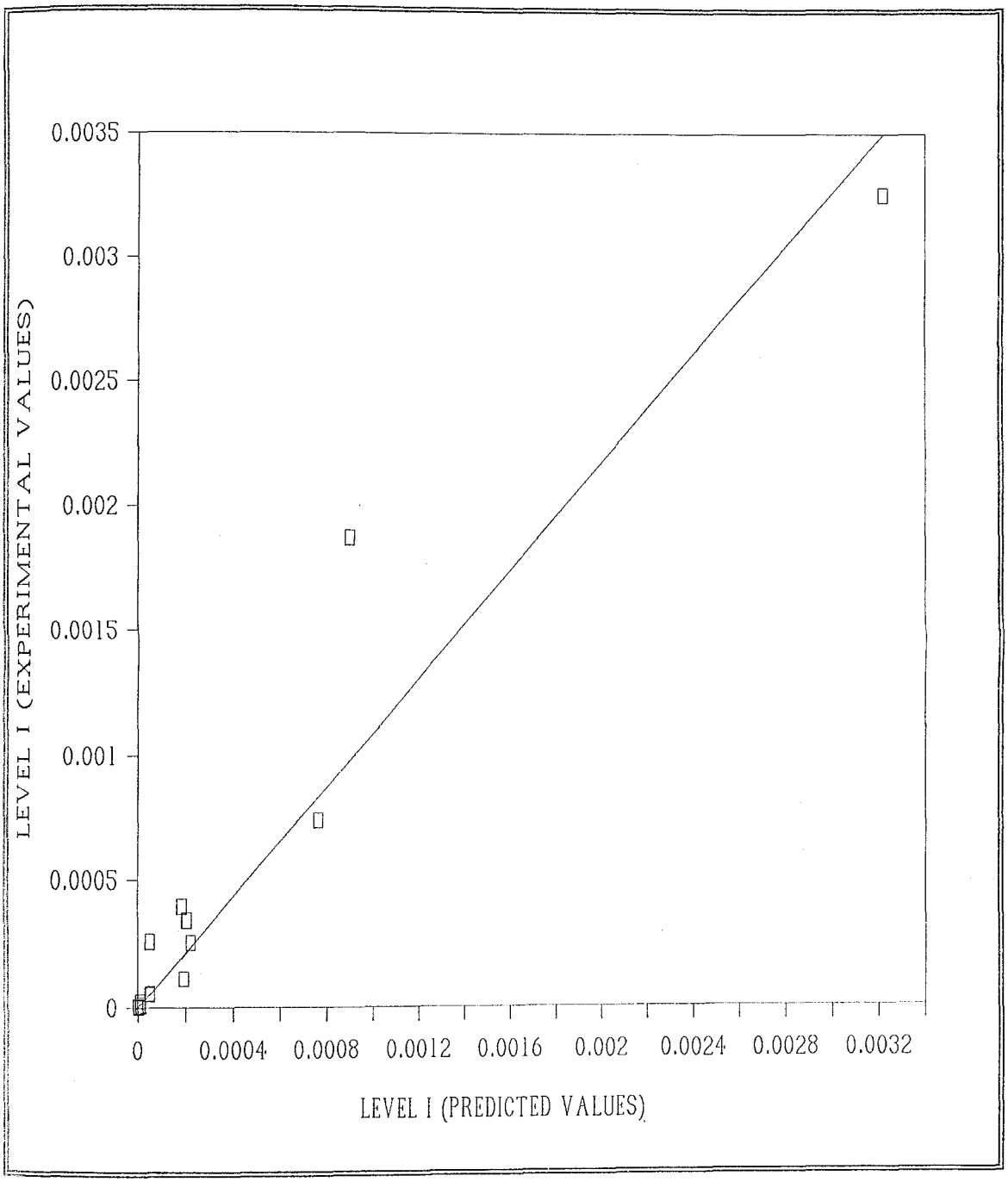

Figure 6.1.1. Equilibrium Distribution (%) in Air.

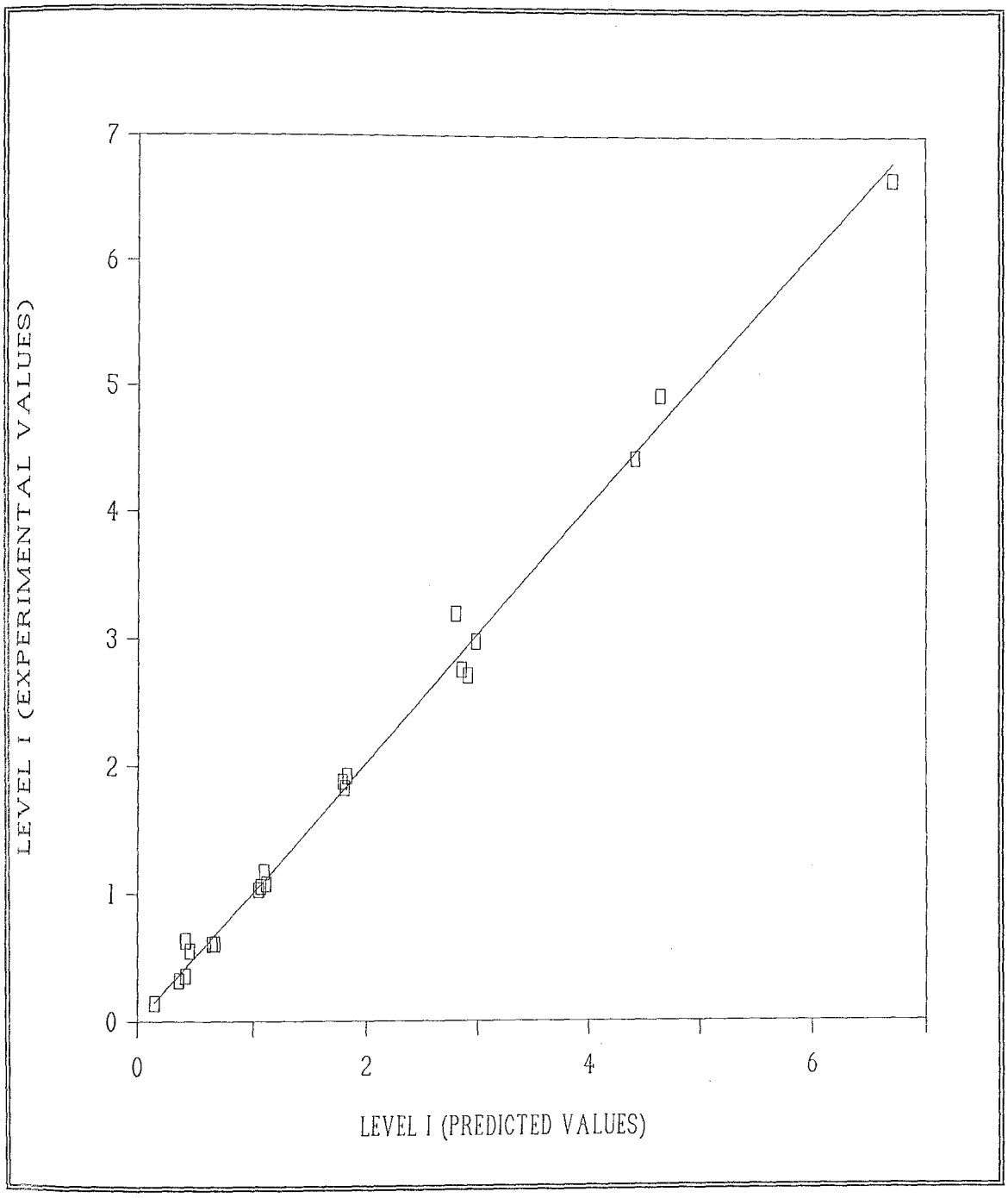

Figure 6.1.2. Equilibrium Distribution (%) in Soil.

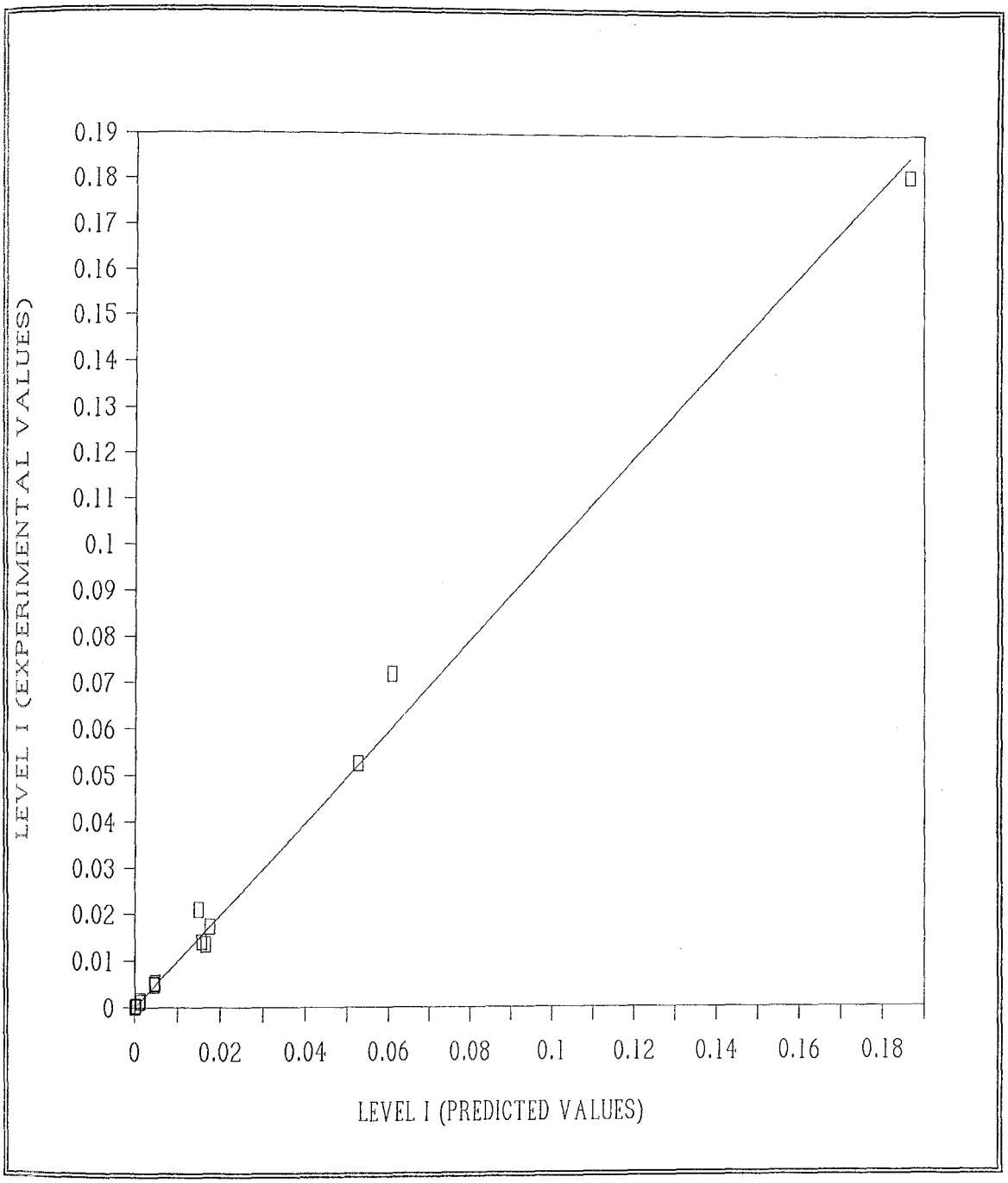

Figure 6.1.3. Equilibrium Distribution (%) in Water.

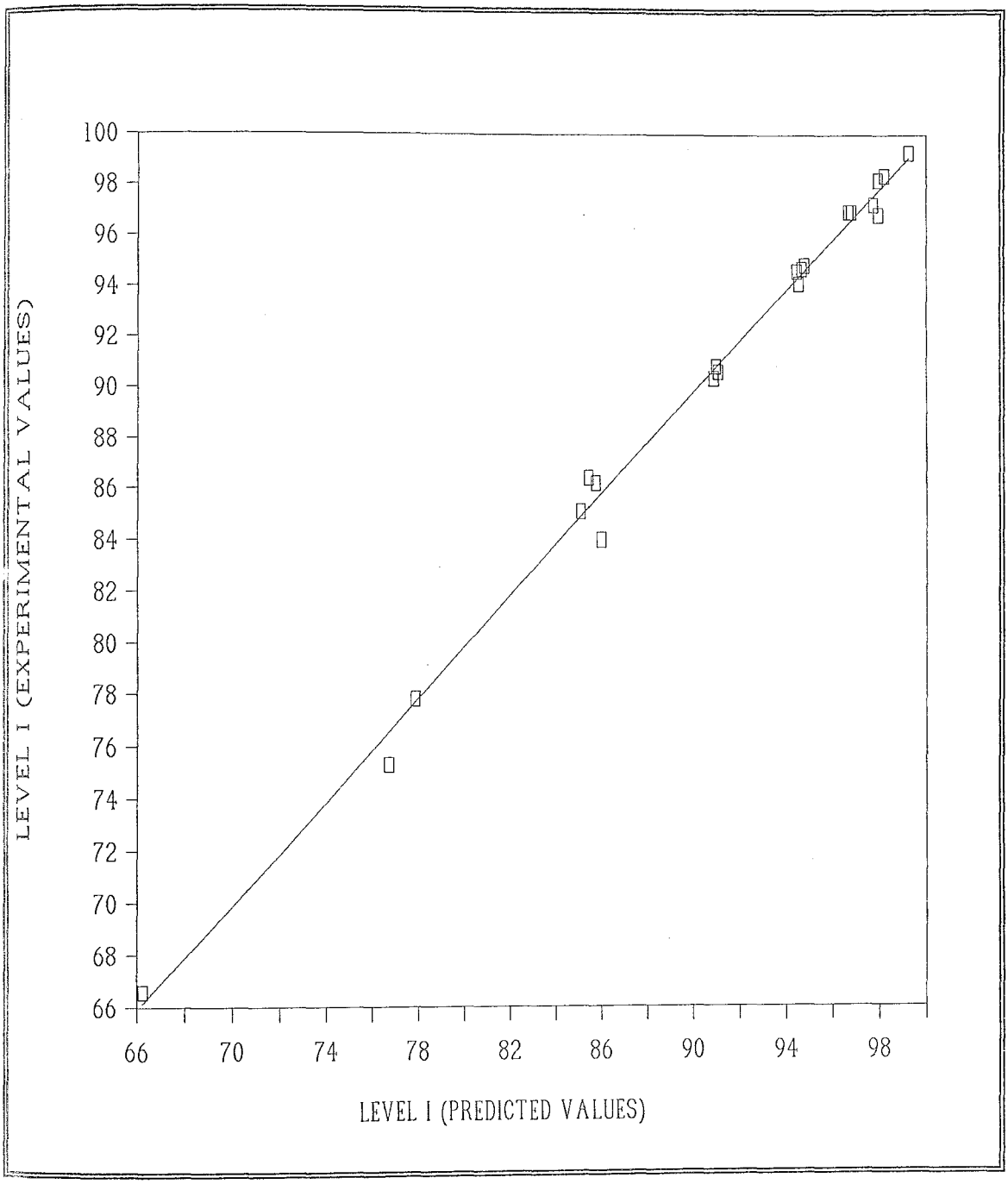

Figure 6.1.4. Equilibrium Distribution (%) in Biota.

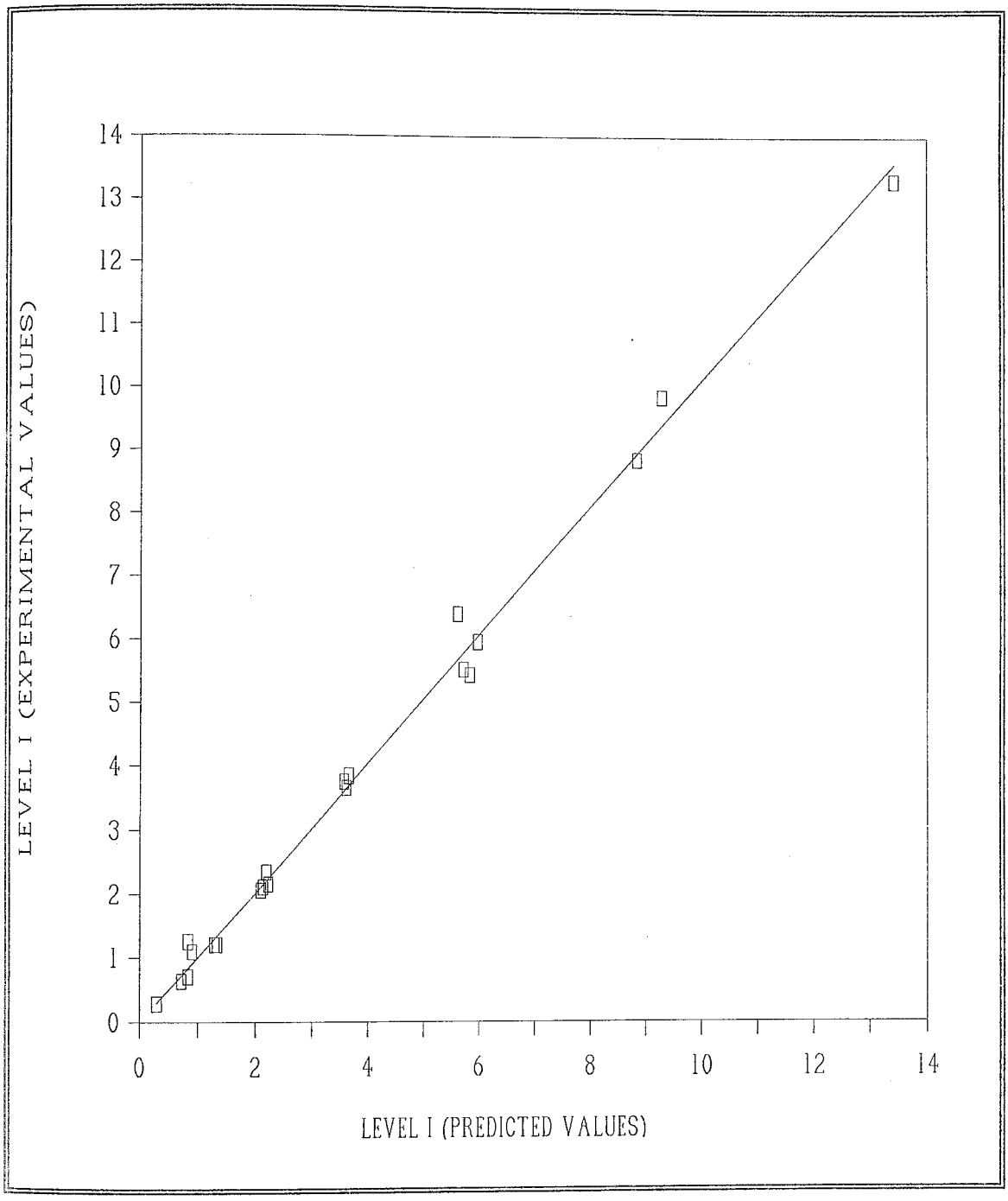

Figure 6.1.5. Equilibrium Distribution (%) in Suspended Solids and Sediment.

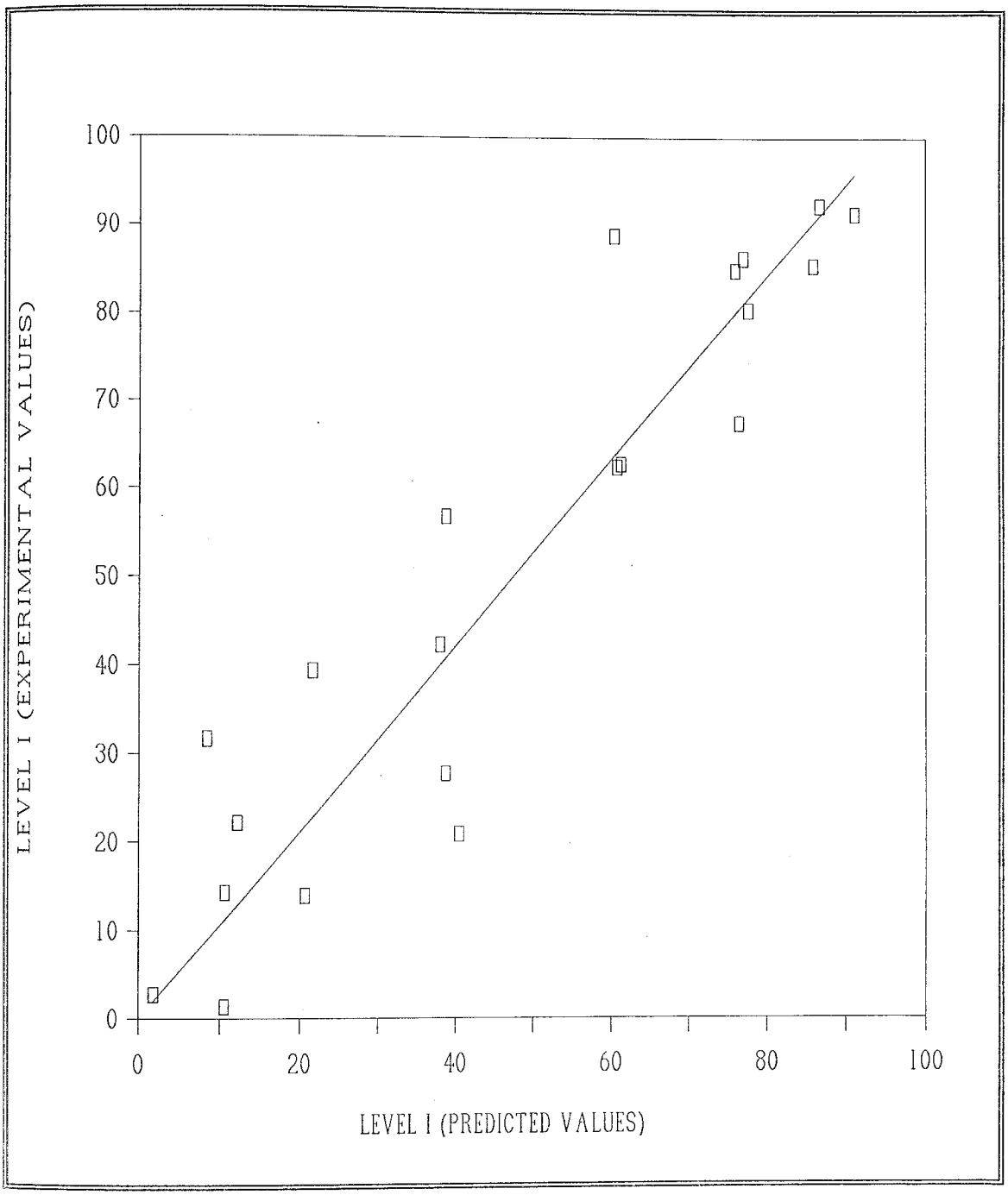

Figure 6.2.1.Mass Distribution (%) in Air.

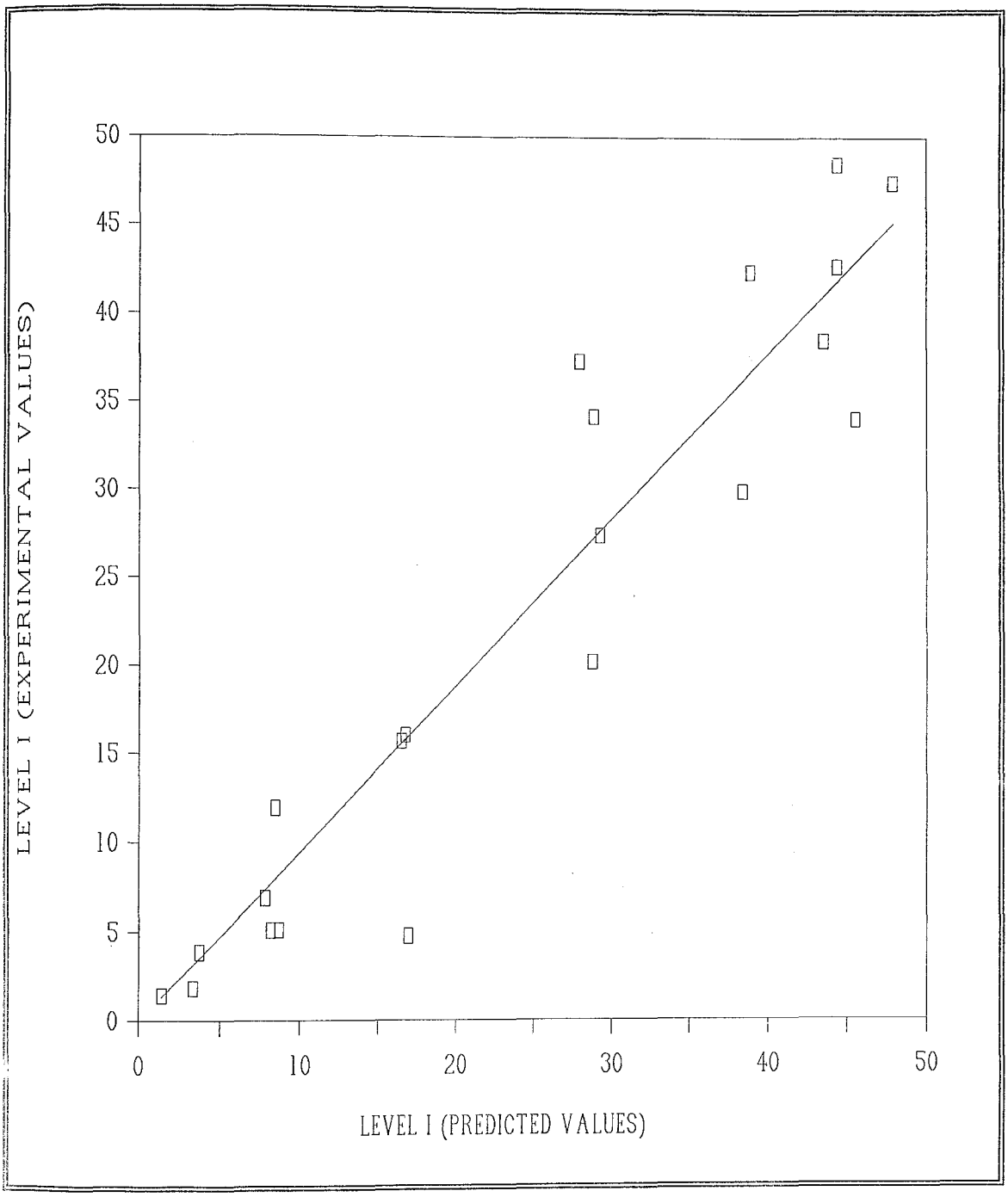

Figure 6.2.2.Mass Distribution (%) in Soil.

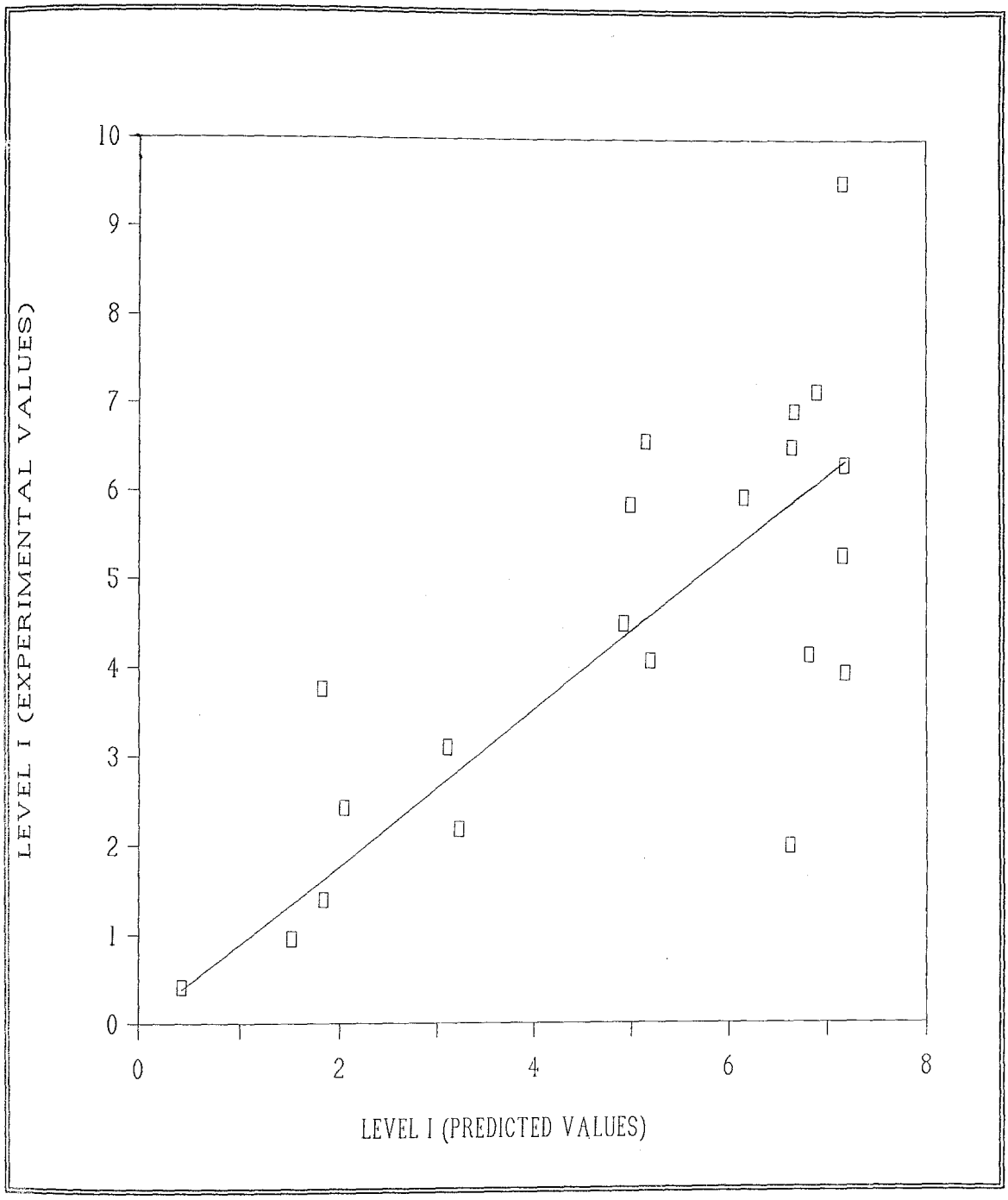

Figure 6.2.3. Mass Distribution (%) in Water.

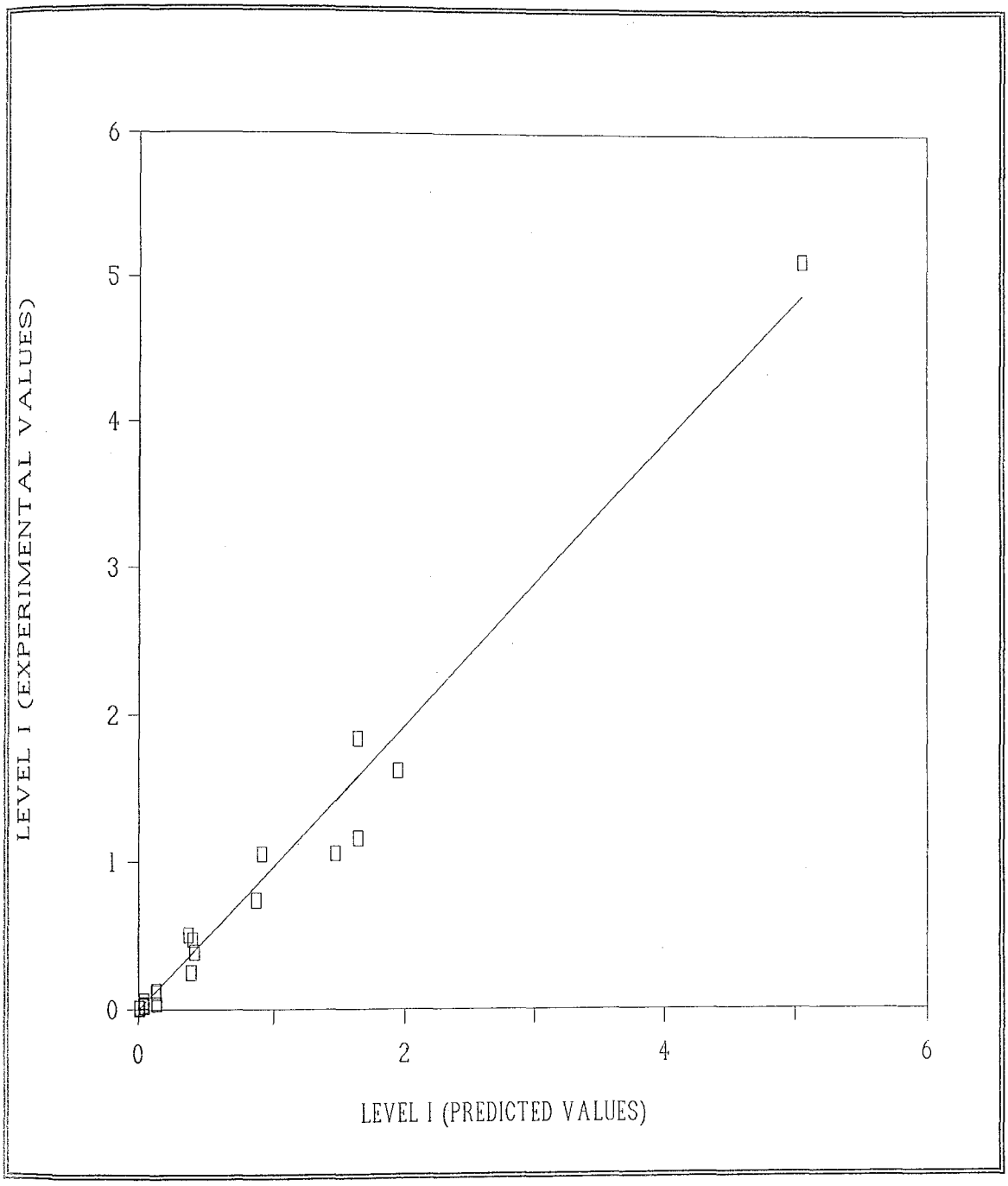

Figure 6.2.4. Mass Distribution (%) in Biota.

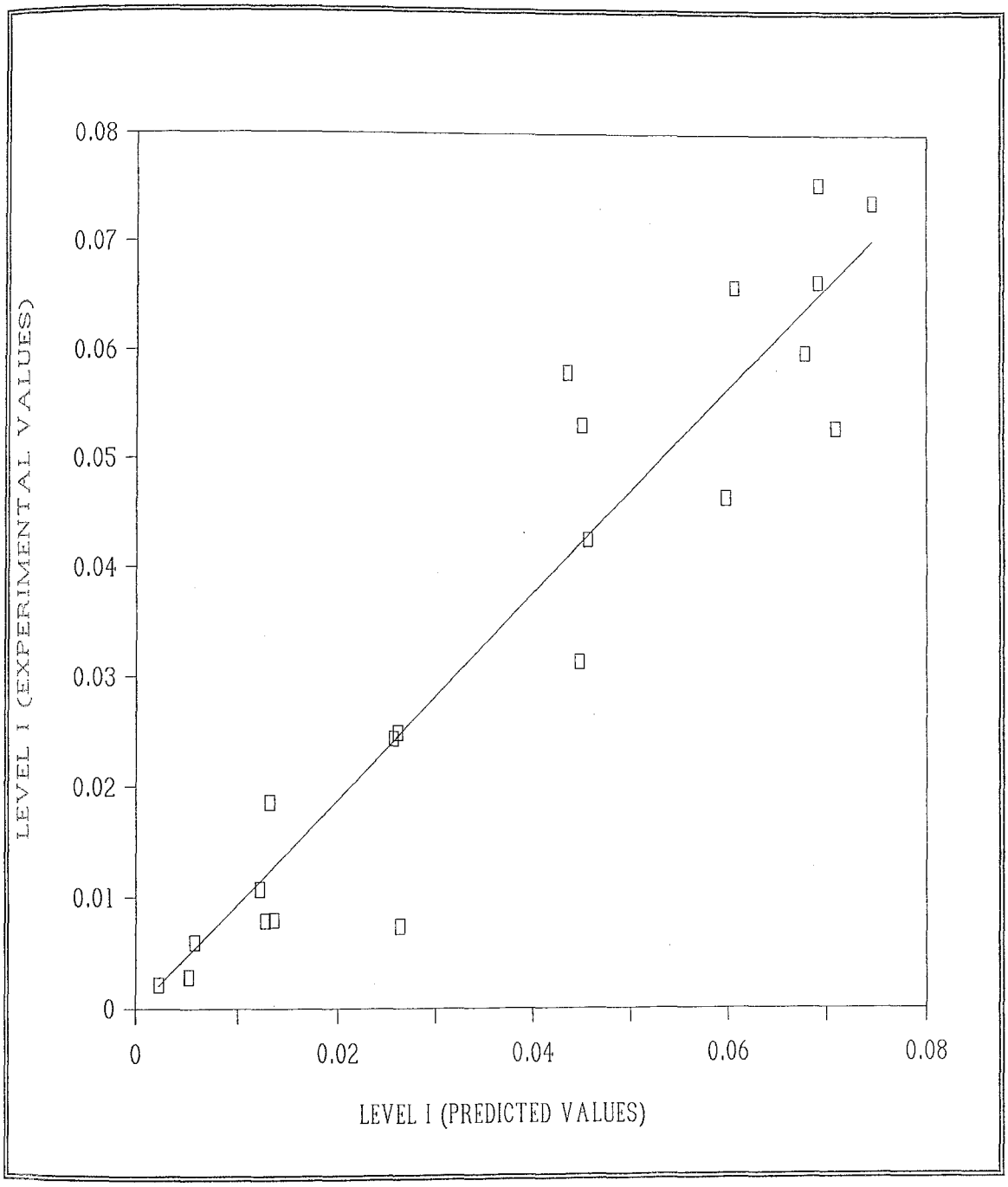

Figure 6.2.5, Mass Distribution (%) in Suspended Solids.

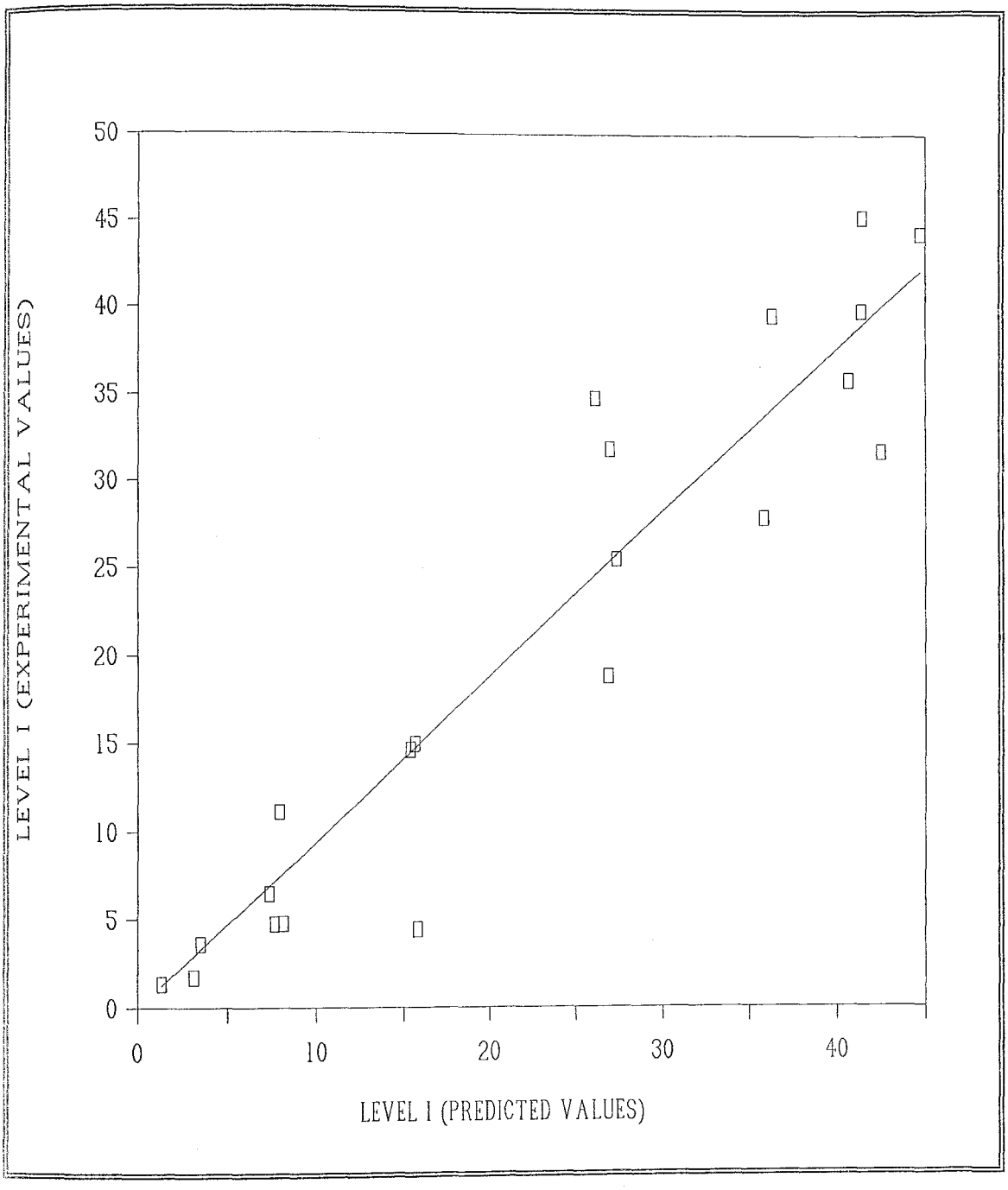

Figure 6.2.6.Mass Distribution (%) in Sediment.

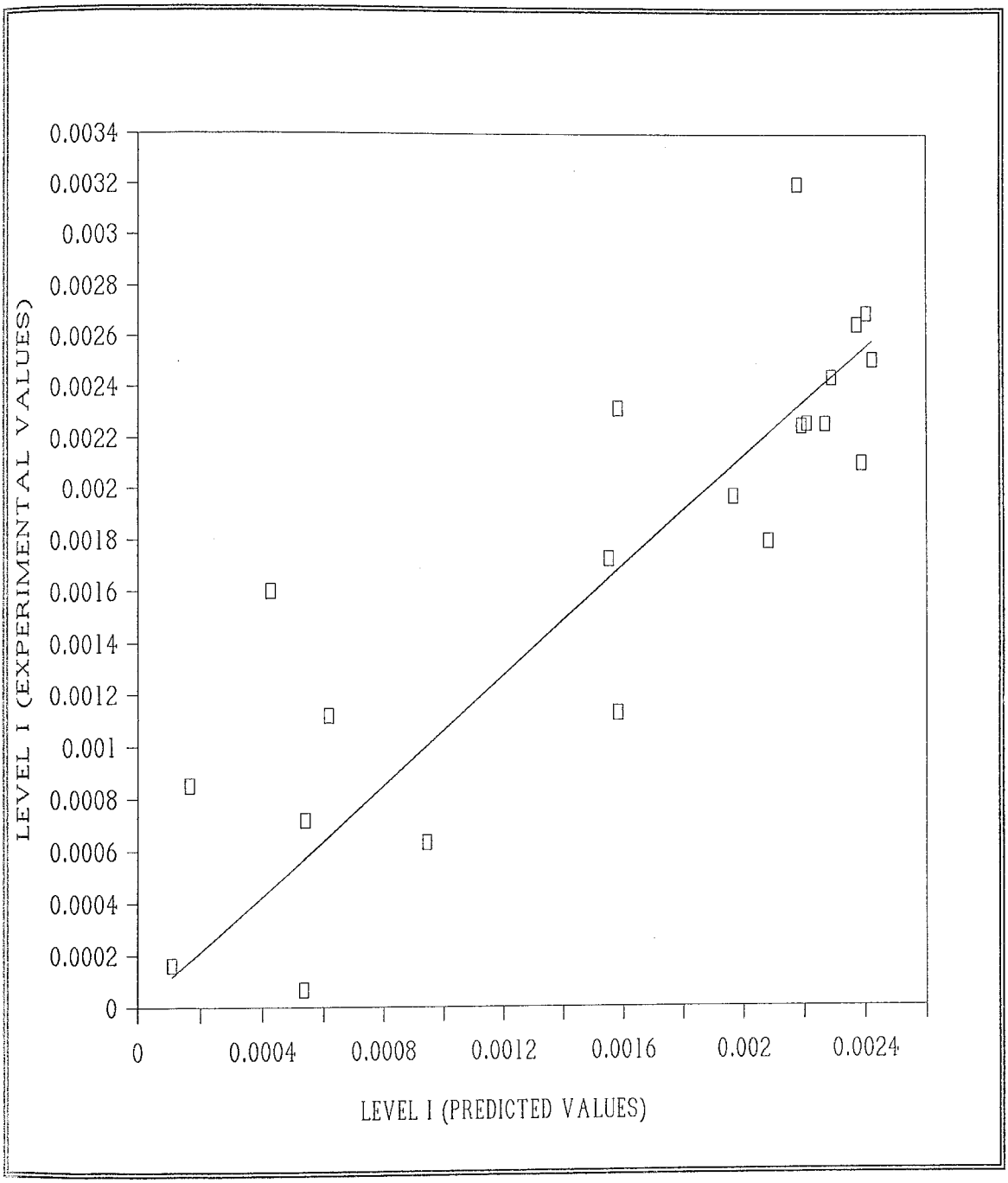

Figure 6.3.1. Concentration (ppm) in Air.

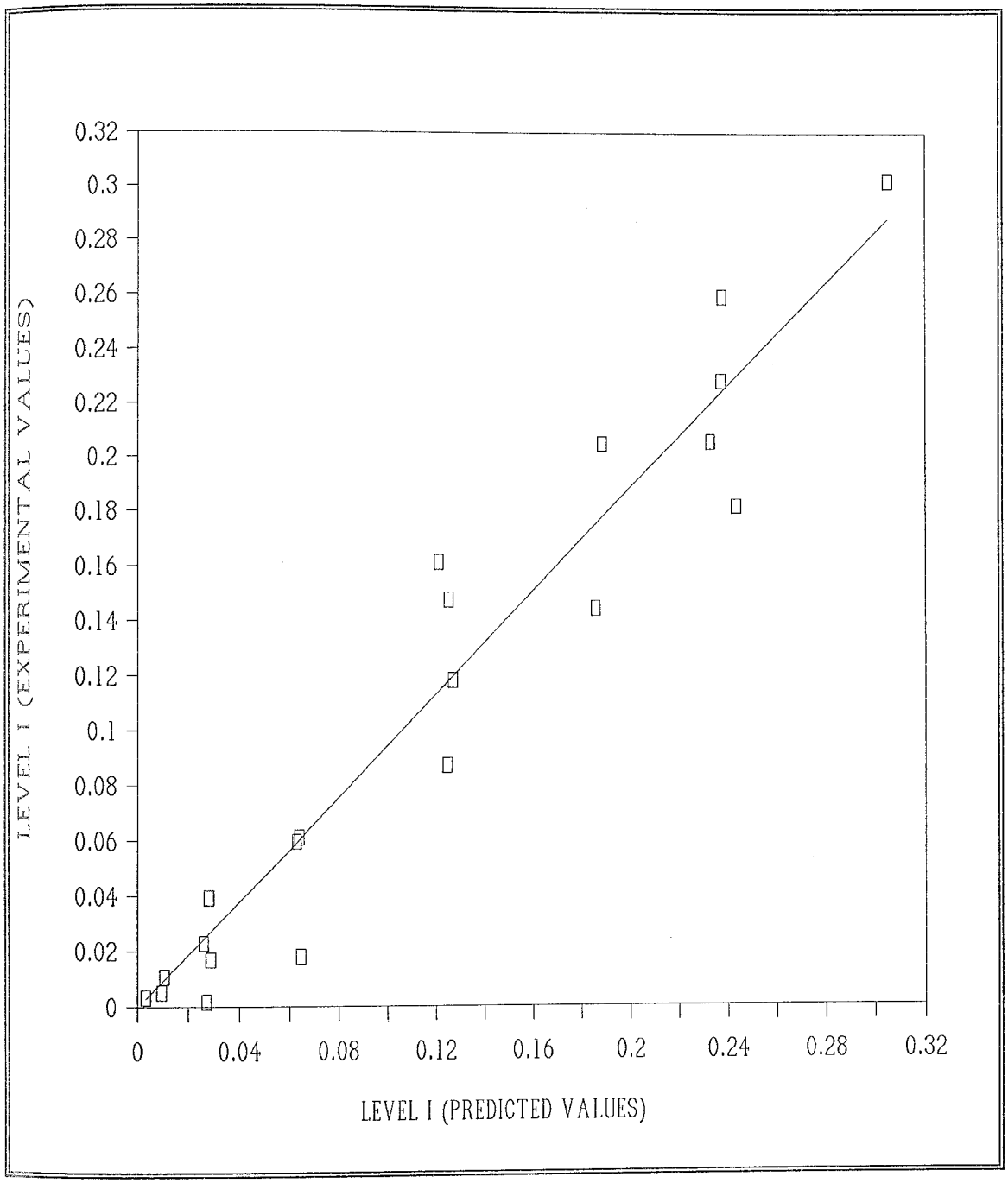

Figure 6.3.2. Concentration (ppm) in Soil.

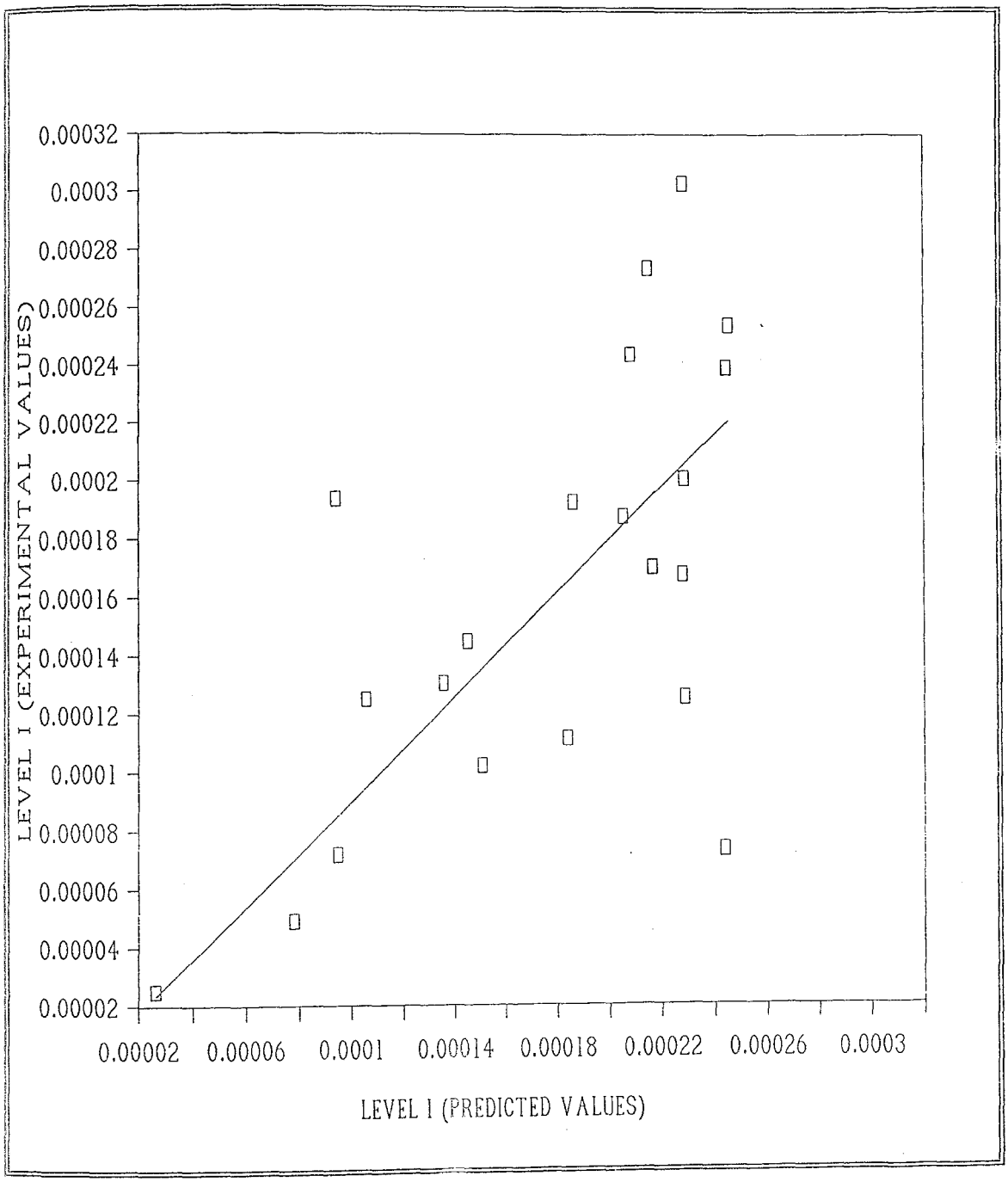

Figure 6.3.3. Concentration (ppm) in Water.

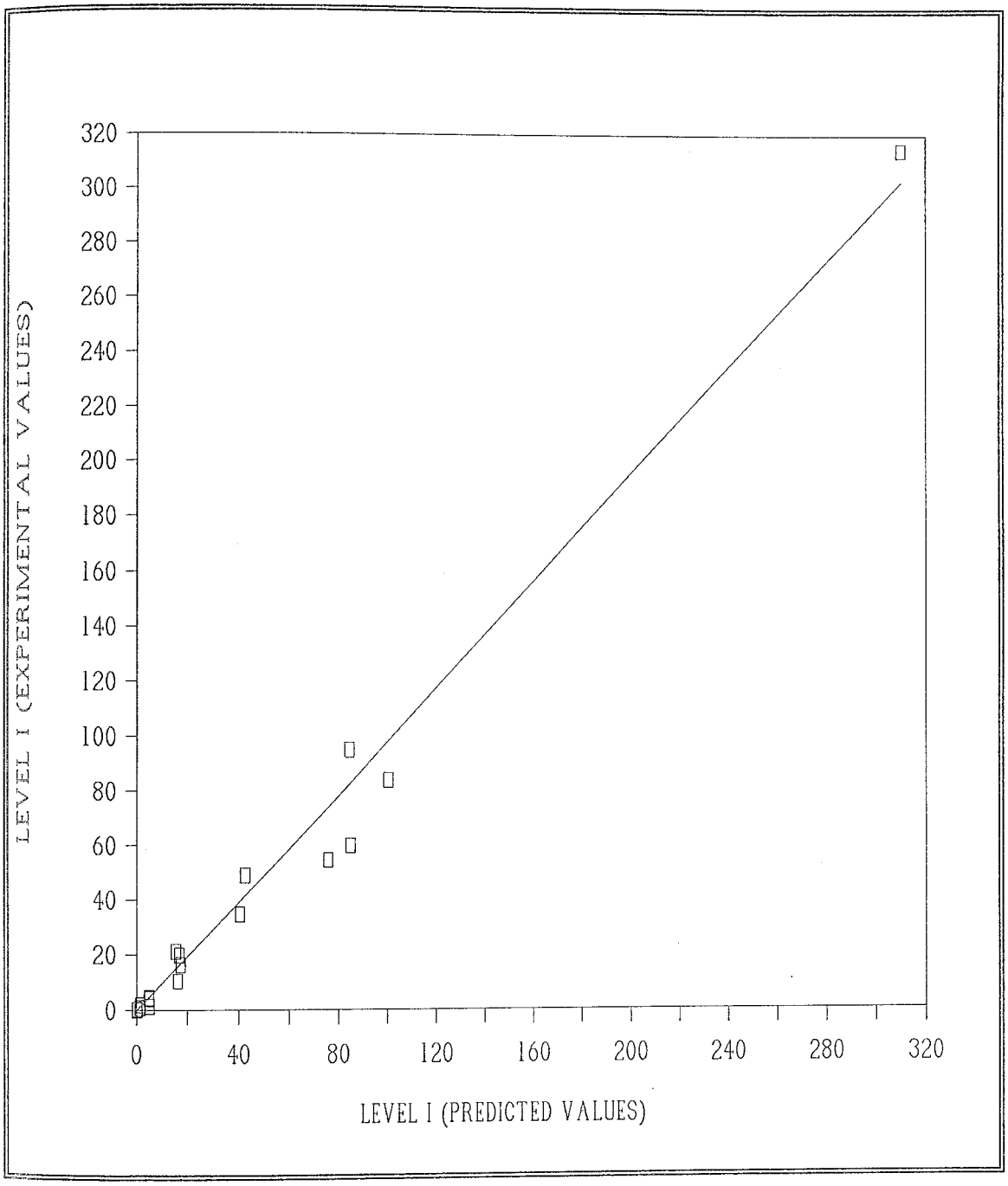

Figure 6.3.4. Concentration (ppm) in Biota.

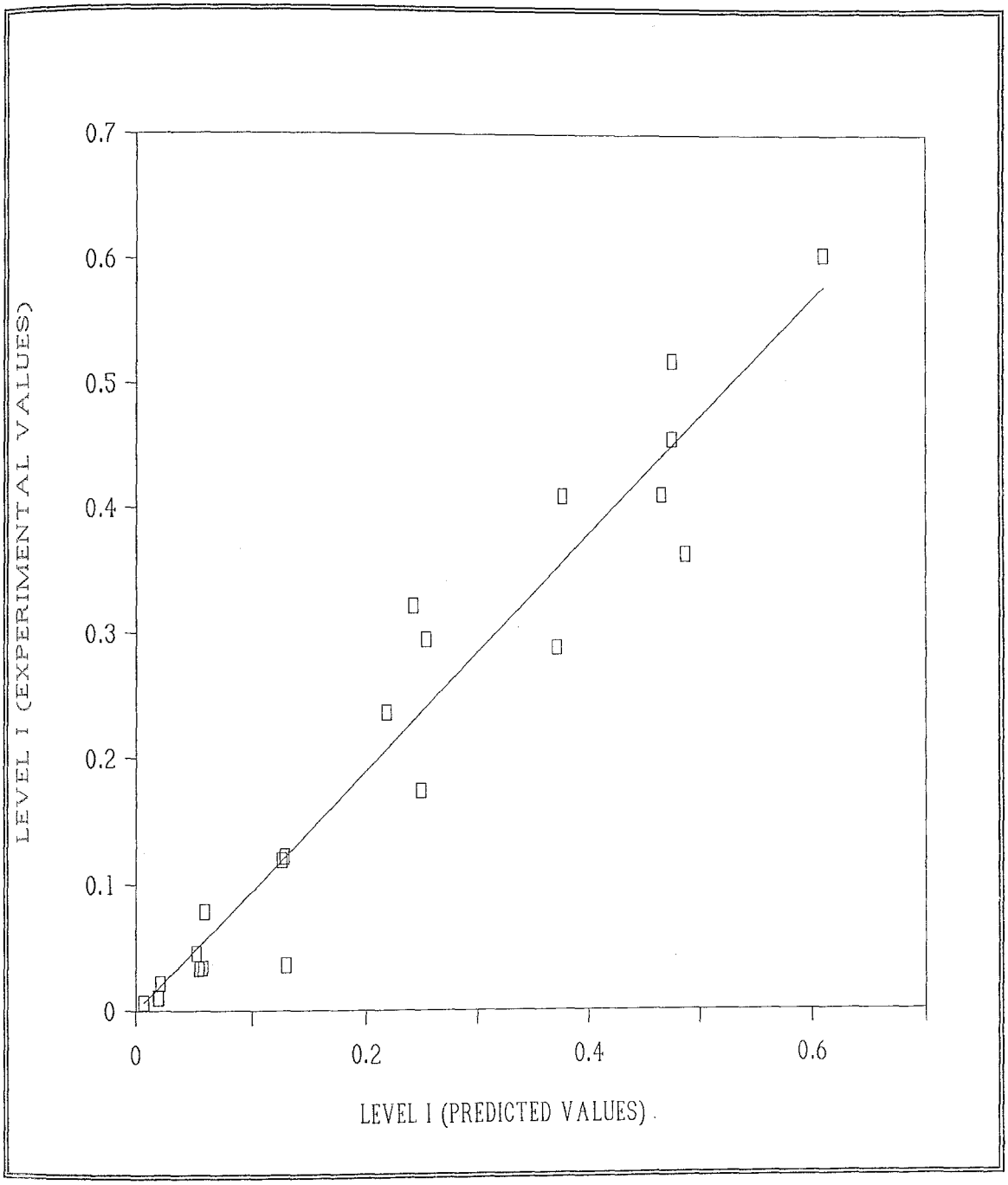

Figure 6.3.5.Concentration (ppm) in Suspended Solids and Sediment.

6.4. CONCLUSION

In this study , it has been demonstrated that a model based on topological properties of a molecule can be used to accurately predict the environmentally important properties of chemicals that constitute a major environmental hazard: PCBs. Measurement of properties such as water solubility, vapour pressure and octanol-water partition coefficients are laborious and time consuming when large numbers of compounds are being considered. Under such conditions, estimation of these properties from structural information such as using the CR index model is advantageous. Calculation of the CR index necessitates the use of a computer; it is difficult to calculate it by hand or a simple calculator. However, with the increasing availability of computing power, for chemical and biochemical research and the growing tendency toward computer storage of structure- property data, the use of techniques such as automatic handling of chemical structure by computer can become widespread.

The approach used herein for the estimation of physicochemical properties is a combination of topological characteristics of the molecule and reported experimental properties in correlation. A significant linear relationship exists between the logarithm of water solubility, vapour pressure, octanol-water partition coefficient and the CR index for PCBs. In fact, nearly 95% accuracy in the prediction of physicochemical properties of PCBs whose physicochemical properties have been measured is possible. This result gives a confidence that this model can also be used in the future predictions of compounds whose physicochemical properties have

not been measured yet.

This approach may be applicable to other series of organic compounds. Accurate physicochemical property determinations are very desirable for which serious discrepancies exist between reported and correlated values. However, in this topological index, certain types of structural information can not be encoded; for instance, structural information of a steric nature such as cis/trans isomerism or chirality can not be reflected in the values of the CR index derived in this study.

On the other hand, such an accurate model can be used to predict the potential environmental hazard of chemicals even before the compounds are synthesized. The establishment of regression equations is a useful and convenient method for extending the existing data bases on the distribution of environmentally important pollutants. These data are used in an evaluative model to asses the fate of PCBs in a Unit World Volume. Depending on the data available, the simplest version of Mackay's Models is extended to provide an estimate of the Potential Environmental Distribution of PCBs under equilibrium conditions. However, the limitations of Mackay's Level I Fugacity Model should be restated. The technique is only applicable to a set of well-defined organic structures. For example, it would be meaningless to attempt an analysis of chemicals such as inorganics, polymers or formulations. The other limitation is that the model is based on the equilibrium situation and says nothing about the kinetics involved in the transfer processes from one medium to another. It presents a picture of the ultimate distribution of a persistent substance in the environment in

terms of both relative concentrations and relative masses.

Nevertheless, using this model, it is possible to set priorities and suggest new directions for the continuing investigation of potential problems associated with chemicals that have or will be introduced into the environment.

As a result, in the future, the CR index may also be helpful in developing new ecological models that will give more insight into the expected distribution of chemicals in the environment. Since the CR index is found to correlate with input data of Model I it is possible from the CR index alone to evaluate the overall distribution of chemicals in the ecosystem. So, the model provides comparative exposure information about chemicals and assists priority settings.

Finally, in order to complete the environmental picture and make a hazard assessment, the exposure prediction should be combined with expected use patterns, toxicity and persistence, such as hydrolysis and photodegradability. This can be the subject of another research.

APPENDIX I

BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.0000	0.3333	0.1667	0.0962	0.1925	0.3333	0.0833	0.0481	0.0278	0.0160	0.0278	0.0481
2	0.3333	0.0000	0.2887	0.1667	0.0962	0.1925	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833
3	0.1667	0.2887	0.0000	0.2887	0.1667	0.0962	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443
4	0.1111	0.1667	0.2887	0.0000	0.3333	0.1925	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833
5	0.1925	0.1111	0.1667	0.3333	0.0000	0.3333	0.0833	0.0481	0.0278	0.0160	0.0278	0.0481
6	0.3333	0.1925	0.0962	0.1925	0.3333	0.0000	0.0481	0.0278	0.0160	0.0093	0.0160	0.0278
7	0.0833	0.1443	0.2500	0.1443	0.0833	0.0481	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887
8	0.0481	0.0833	0.1443	0.0833	0.0481	0.0278	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667
9	0.0278	0.0481	0.0833	0.0481	0.0278	0.0160	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111
10	0.0160	0.0278	0.0481	0.0278	0.0160	0.0093	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925
11	0.0278	0.0481	0.0833	0.0481	0.0481	0.0278	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333
12	0.0481	0.0833	0.1443	0.0833	0.0481	0.0278	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000

2-CHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.0000	0.2887	0.1443	0.0833	0.1925	0.3333	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.3475
2	0.2887	0.0000	0.2500	0.1443	0.0833	0.1667	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.6019
3	0.1443	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.3010
4	0.1111	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.1738
5	0.1925	0.0962	0.1667	0.3333	0.0000	0.3333	0.0833	0.0481	0.0278	0.0160	0.0278	0.0481	0.1158
6	0.3333	0.1667	0.0833	0.1925	0.3333	0.0000	0.0417	0.0241	0.0139	0.0080	0.0139	0.0241	0.2006
7	0.0722	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.1505
8	0.0417	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.0000	0.3333	0.1925	0.3333	0.1667	0.0869
9	0.0241	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0502
10	0.0139	0.0241	0.0481	0.0278	0.0160	0.0093	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0290
11	0.0241	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0502
12	0.0417	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0869
13	0.3475	0.6019	0.3010	0.1738	0.1003	0.2006	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.0000

4-CHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.0000	0.3333	0.1667	0.0962	0.1667	0.2887	0.0833	0.0481	0.0278	0.0160	0.0278	0.0481	0.3475
2	0.3333	0.0000	0.2887	0.1667	0.0962	0.1667	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.2006
3	0.1667	0.2887	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1003
4	0.0962	0.1667	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.2006
5	0.1667	0.0962	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0278	0.0160	0.0278	0.0481	0.3475
6	0.2887	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0241	0.0139	0.0080	0.0139	0.0241	0.6019
7	0.0833	0.1443	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.0502
8	0.0481	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0290
9	0.0278	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0167
10	0.0160	0.0278	0.0481	0.0278	0.0160	0.0080	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0097
11	0.0278	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0167
12	0.0481	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0290
13	0.3475	0.2006	0.1003	0.2006	0.3475	0.6019	0.0502	0.0290	0.0167	0.0097	0.0167	0.0290	0.0000

2-2'-DICHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.0000	0.2887	0.1443	0.0833	0.1925	0.3333	0.0722	0.0361	0.0208	0.0139	0.0241	0.0417	0.3475	0.0434
2	0.2887	0.0000	0.2500	0.1443	0.0833	0.1667	0.1250	0.0625	0.0361	0.0241	0.0417	0.0722	0.6019	0.0752
3	0.1443	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1250	0.0722	0.0481	0.0833	0.1443	0.3010	0.1505
4	0.1111	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0722	0.0417	0.0278	0.0481	0.0833	0.1738	0.0869
5	0.1925	0.1132	0.1667	0.3333	0.0000	0.3333	0.0833	0.0417	0.0241	0.0139	0.0278	0.0481	0.1363	0.0502
6	0.3333	0.1667	0.0833	0.1925	0.3333	0.0000	0.0417	0.0208	0.0120	0.0069	0.0139	0.0241	0.2006	0.0251
7	0.0722	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2500	0.1443	0.0833	0.1667	0.2887	0.1505	0.3010
8	0.0361	0.0625	0.1250	0.0722	0.0417	0.0241	0.2500	0.0000	0.2887	0.1667	0.0962	0.1443	0.0752	0.6019
9	0.0208	0.0361	0.0722	0.0417	0.0241	0.0139	0.1443	0.2887	0.0000	0.3333	0.1925	0.1111	0.0434	0.3475
10	0.0139	0.0241	0.0481	0.0278	0.0160	0.0093	0.0962	0.1667	0.3333	0.0000	0.3333	0.1925	0.0290	0.2006
11	0.0241	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.0833	0.1925	0.3333	0.0000	0.3333	0.0502	0.1003
12	0.0417	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1443	0.0833	0.1925	0.3333	0.0000	0.0869	0.1738
13	0.3475	0.6019	0.3010	0.1738	0.1003	0.2006	0.1505	0.0752	0.0434	0.0290	0.0502	0.0869	0.0000	0.0906
14	0.0434	0.0752	0.1505	0.0869	0.0502	0.0290	0.3010	0.6019	0.3475	0.2006	0.1158	0.1738	0.0906	0.0000

4-4'-DICHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.0000	0.3333	0.1667	0.0962	0.1667	0.2500	0.0833	0.0481	0.0278	0.0139	0.0278	0.0481	0.3010	0.0167
2	0.3333	0.0000	0.2887	0.1667	0.0962	0.1667	0.1443	0.0833	0.0481	0.0241	0.0481	0.0833	0.2006	0.0290
3	0.1667	0.2887	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0833	0.0417	0.0833	0.1443	0.1003	0.0502
4	0.0962	0.1667	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0481	0.0241	0.0481	0.0833	0.2006	0.0290
5	0.1667	0.0962	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0278	0.0139	0.0278	0.0481	0.3475	0.0167
6	0.2500	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0241	0.0139	0.0069	0.0139	0.0241	0.6019	0.0084
7	0.0833	0.1443	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.0502	0.1003
8	0.0481	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0290	0.2006
9	0.0278	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0167	0.3475
10	0.0139	0.0241	0.0417	0.0241	0.0139	0.0069	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0084	0.6019
11	0.0278	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0167	0.3475
12	0.0481	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0290	0.2006
13	0.3010	0.2006	0.1003	0.2006	0.3475	0.6019	0.0502	0.0290	0.0167	0.0084	0.0167	0.0290	0.0000	0.0101
14	0.0167	0.0290	0.0502	0.0290	0.0167	0.0084	0.1003	0.2006	0.3475	0.6019	0.3475	0.2006	0.0101	0.0000

2-5-DICHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.3333	0.0722	0.0417	0.0241	0.0139	0.0241	0.0241	0.2006	0.3475
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1667	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.0869	0.6019
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0833	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1738	0.3010
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.3475	0.1738
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.6019	0.1003
6	0.3333	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0241	0.0139	0.0080	0.0139	0.0241	0.3475	0.2006
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0417	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.0869	0.1505
8	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0502	0.0869
9	0.0241	0.0417	0.0833	0.0481	0.0241	0.0139	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0290	0.0502
10	0.0139	0.0241	0.0481	0.0278	0.0139	0.0080	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0167	0.0290
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0139	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0290	0.0502
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0502	0.0869
13	0.2006	0.1003	0.1738	0.3475	0.6019	0.3475	0.0869	0.0502	0.0290	0.0167	0.0290	0.0502	0.0000	0.1208
14	0.3475	0.6019	0.3010	0.1738	0.0869	0.2006	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.1046	0.0000

2-6- DICHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.0000	0.2887	0.1443	0.0722	0.1925	0.3333	0.0722	0.0417	0.0241	0.0139	0.0241	0.0241	0.0869	0.3475
2	0.2887	0.0000	0.2500	0.1250	0.0722	0.1667	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.1505	0.6019
3	0.1443	0.2500	0.0000	0.2500	0.1443	0.0833	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.3010	0.3010
4	0.0962	0.1250	0.2500	0.0000	0.2887	0.1667	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.6019	0.1505
5	0.1925	0.0962	0.1443	0.2887	0.0000	0.3333	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.3475	0.1158
6	0.3333	0.1667	0.0833	0.1667	0.3333	0.0000	0.0417	0.0241	0.0139	0.0080	0.0139	0.0241	0.2006	0.2006
7	0.0722	0.1250	0.2500	0.1250	0.0722	0.0417	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.1505	0.1505
8	0.0417	0.0722	0.1443	0.0722	0.0417	0.0241	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0869	0.0869
9	0.0241	0.0417	0.0833	0.0417	0.0241	0.0139	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0502	0.0502
10	0.0139	0.0241	0.0481	0.0241	0.0139	0.0080	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0290	0.0290
11	0.0241	0.0417	0.0833	0.0417	0.0241	0.0139	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0502	0.0502
12	0.0417	0.0722	0.1443	0.0722	0.0417	0.0241	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0869	0.0869
13	0.1158	0.1505	0.3010	0.6019	0.3475	0.2006	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.0000	0.1812
14	0.3475	0.6019	0.3010	0.1505	0.0869	0.2006	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.1812	0.0000

2-4'-DICHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.0000	0.2887	0.1443	0.0833	0.1925	0.3333	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.3475	0.0167
2	0.2887	0.0000	0.2500	0.1443	0.0833	0.1667	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.6019	0.0290
3	0.1443	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.3010	0.0579
4	0.1111	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.1738	0.0334
5	0.1925	0.0962	0.1667	0.3333	0.0000	0.3333	0.0833	0.0481	0.0278	0.0139	0.0278	0.0481	0.1158	0.0167
6	0.3333	0.1667	0.0833	0.1925	0.3333	0.0000	0.0417	0.0241	0.0139	0.0069	0.0139	0.0241	0.2006	0.0084
7	0.0722	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.1505	0.1003
8	0.0417	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0869	0.2006
9	0.0241	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0502	0.3475
10	0.0139	0.0241	0.0481	0.0278	0.0160	0.0093	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0290	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0502	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0869	0.2006
13	0.3475	0.6019	0.3010	0.1738	0.1003	0.2006	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.0000	0.0302
14	0.0167	0.0290	0.0579	0.0334	0.0193	0.0111	0.1003	0.2006	0.3475	0.6019	0.3475	0.2006	0.0302	0.0000

3-4-DICHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2500	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.6019	0.3010
2	0.2887	0.0000	0.2887	0.1667	0.0962	0.1443	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.3475	0.1738
3	0.1443	0.2887	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1738	0.1003
4	0.0833	0.1667	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.1003	0.2006
5	0.2500	0.1443	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0278	0.0160	0.0278	0.0481	0.3010	0.3475
6	0.2500	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0208	0.0120	0.0069	0.0120	0.0208	0.3010	0.6019
7	0.0722	0.1443	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.0869	0.0502
8	0.0417	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0502	0.0290
9	0.0241	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0290	0.0167
10	0.0139	0.0278	0.0481	0.0278	0.0160	0.0080	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0167	0.0097
11	0.0241	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0290	0.0167
12	0.0417	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0502	0.0290
13	0.6019	0.3475	0.1738	0.1003	0.1738	0.3010	0.0869	0.0502	0.0290	0.0167	0.0290	0.0502	0.0000	0.3623
14	0.3010	0.1738	0.0869	0.2006	0.3475	0.6019	0.0434	0.0251	0.0145	0.0084	0.0145	0.0251	0.3623	0.0000

3-3'-DICHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.2887	0.0722	0.0417	0.0208	0.0120	0.0241	0.0417	0.6019	0.0251
2	0.2887	0.0000	0.2887	0.1667	0.0962	0.1667	0.1443	0.0833	0.0417	0.0241	0.0481	0.0833	0.3475	0.0502
3	0.1443	0.2887	0.0000	0.2887	0.1667	0.0962	0.2500	0.1443	0.0722	0.0754	0.0833	0.1443	0.1738	0.0869
4	0.0962	0.1667	0.2887	0.0000	0.3333	0.1925	0.1443	0.0833	0.0417	0.0241	0.0481	0.0833	0.1158	0.0502
5	0.1667	0.0962	0.1667	0.3333	0.0000	0.3333	0.0833	0.0481	0.0241	0.0139	0.0278	0.0481	0.2006	0.0290
6	0.2887	0.1667	0.0833	0.1925	0.3333	0.0000	0.0417	0.0241	0.0120	0.0069	0.0139	0.0241	0.3475	0.0145
7	0.0722	0.1443	0.2500	0.1443	0.0833	0.0481	0.0000	0.2887	0.1443	0.0833	0.1667	0.2887	0.0869	0.1738
8	0.0417	0.0833	0.1443	0.0833	0.0481	0.0278	0.2887	0.0000	0.2887	0.1667	0.0962	0.1667	0.0502	0.3475
9	0.0208	0.0417	0.0722	0.0417	0.0241	0.0139	0.1443	0.2887	0.0000	0.2887	0.1667	0.0962	0.0251	0.6019
10	0.0139	0.0278	0.0481	0.0278	0.0160	0.0093	0.0962	0.1667	0.2887	0.0000	0.3333	0.1925	0.0167	0.3475
11	0.0241	0.0481	0.0833	0.0481	0.0278	0.0160	0.1667	0.0962	0.1667	0.3333	0.0000	0.3333	0.0290	0.2006
12	0.0417	0.0833	0.1443	0.0833	0.0481	0.0278	0.2887	0.1667	0.0833	0.1925	0.3333	0.0000	0.0502	0.1003
13	0.6019	0.3475	0.1738	0.1003	0.2006	0.3475	0.0869	0.0502	0.0251	0.0145	0.0290	0.0502	0.0000	0.0302
14	0.0251	0.0502	0.0869	0.0502	0.0290	0.0167	0.1738	0.3475	0.4201	0.3475	0.2006	0.1158	0.0302	0.0000

2-2'-3-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2500	0.1250	0.0722	0.1667	0.2887	0.0625	0.0313	0.0180	0.0104	0.0208	0.0361	0.6019	0.3010	0.0376
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0625	0.0361	0.0208	0.0417	0.0722	0.3010	0.6019	0.0752
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1250	0.0722	0.0417	0.0833	0.1443	0.1505	0.3010	0.1505
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0722	0.0417	0.0241	0.0481	0.0833	0.1158	0.1738	0.0869
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.3333	0.0833	0.0417	0.0241	0.0139	0.0278	0.0481	0.2006	0.1003	0.0502
6	0.2887	0.1443	0.0695	0.1925	0.3333	0.0000	0.0361	0.0180	0.0104	0.0060	0.0120	0.0208	0.3475	0.1738	0.0217
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2500	0.1443	0.0833	0.1667	0.2887	0.0752	0.1505	0.3010
8	0.0313	0.0625	0.1250	0.0722	0.0417	0.0241	0.2500	0.0000	0.2887	0.1667	0.0962	0.1443	0.0376	0.0752	0.6019
9	0.0180	0.0361	0.0722	0.0417	0.0241	0.0139	0.1443	0.2887	0.0000	0.3333	0.1925	0.1111	0.0217	0.0434	0.3475
10	0.0120	0.0241	0.0481	0.0278	0.0160	0.0093	0.0962	0.1667	0.3333	0.0000	0.3333	0.1925	0.0145	0.0290	0.2006
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.0833	0.1925	0.3333	0.0000	0.3333	0.0251	0.0502	0.1003
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1443	0.0833	0.1925	0.3333	0.0000	0.0434	0.0869	0.1738
13	0.6019	0.3010	0.1505	0.0869	0.2006	0.3475	0.0752	0.0376	0.0217	0.0125	0.0251	0.0434	0.0000	0.3623	0.0453
14	0.3010	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0752	0.0434	0.0251	0.0502	0.0869	0.3623	0.0000	0.0906
15	0.0376	0.0752	0.1505	0.0869	0.0502	0.0290	0.3010	0.6019	0.3475	0.2006	0.1158	0.1738	0.0453	0.0906	0.0000

2-2'-4-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.2887	0.0722	0.0361	0.0208	0.0120	0.0241	0.0417	0.3475	0.3475	0.0434
2	0.2887	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0625	0.0361	0.0208	0.0417	0.0722	0.1738	0.6019	0.0752
3	0.1443	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1250	0.0722	0.0417	0.0833	0.1443	0.1003	0.3010	0.1505
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0722	0.0417	0.0241	0.0481	0.0833	0.2006	0.1738	0.0869
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.2887	0.0833	0.0417	0.0241	0.0139	0.0278	0.0481	0.3475	0.1003	0.0502
6	0.2887	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0180	0.0090	0.0060	0.0120	0.0208	0.6019	0.1738	0.0217
7	0.0722	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2500	0.1443	0.0833	0.1667	0.2887	0.0502	0.1505	0.3010
8	0.0361	0.0625	0.1250	0.0722	0.0417	0.0208	0.2500	0.0000	0.2887	0.1667	0.0962	0.1443	0.0251	0.0752	0.6019
9	0.0208	0.0361	0.0722	0.0417	0.0241	0.0120	0.1443	0.2887	0.0000	0.3333	0.1925	0.1111	0.0145	0.0434	0.3475
10	0.0139	0.0241	0.0481	0.0278	0.0160	0.0080	0.0962	0.1667	0.3333	0.0000	0.3333	0.1925	0.0097	0.0290	0.2006
11	0.0241	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0833	0.1925	0.3333	0.0000	0.3333	0.0167	0.0502	0.1003
12	0.0417	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1443	0.0833	0.1925	0.3333	0.0000	0.0290	0.0869	0.1738
13	0.3475	0.1738	0.0869	0.2006	0.3475	0.6019	0.0434	0.0217	0.0109	0.0072	0.0145	0.0251	0.0000	0.2092	0.0261
14	0.3475	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0752	0.0434	0.0251	0.0502	0.0869	0.2092	0.0000	0.0906
15	0.0434	0.0752	0.1505	0.0869	0.0502	0.0251	0.3010	0.6019	0.3475	0.2006	0.1158	0.1738	0.0302	0.0906	0.0000

2-2'-5-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.3333	0.0722	0.0361	0.0208	0.0120	0.0241	0.0417	0.3475	0.2006	0.0434
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1667	0.1250	0.0625	0.0361	0.0208	0.0417	0.0722	0.6019	0.0869	0.0752
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0833	0.2500	0.1250	0.0722	0.0417	0.0833	0.1443	0.3010	0.1738	0.1505
4	0.0962	0.1443	0.2887	0.0000	0.2887	0.1667	0.1443	0.0722	0.0417	0.0241	0.0481	0.0833	0.1738	0.3475	0.0869
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0208	0.0120	0.0241	0.0417	0.1003	0.6019	0.0434
6	0.3333	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0208	0.0120	0.0069	0.0139	0.0241	0.2006	0.3475	0.0251
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0417	0.0000	0.2500	0.1443	0.0833	0.1667	0.2887	0.1505	0.0869	0.3010
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0208	0.2500	0.0000	0.2887	0.1667	0.0962	0.1443	0.0752	0.0434	0.6019
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0120	0.1443	0.2887	0.0000	0.3333	0.1925	0.1111	0.0434	0.0251	0.3475
10	0.0139	0.0241	0.0481	0.0278	0.0139	0.0080	0.0962	0.1667	0.3333	0.0000	0.3333	0.1925	0.0290	0.0167	0.2006
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0139	0.1667	0.0833	0.1925	0.3333	0.0000	0.3333	0.0502	0.0290	0.1003
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.1443	0.0833	0.1925	0.3333	0.0000	0.0869	0.0502	0.1738
13	0.3475	0.6019	0.3010	0.1738	0.0869	0.2006	0.1505	0.0752	0.0434	0.0251	0.0502	0.0869	0.0000	0.1046	0.0906
14	0.2006	0.1003	0.1738	0.3475	0.6019	0.3475	0.0869	0.0434	0.0251	0.0145	0.0290	0.0502	0.1208	0.0000	0.0523
15	0.0434	0.0752	0.1505	0.0869	0.0434	0.0251	0.3010	0.6019	0.3475	0.2006	0.1158	0.1738	0.0906	0.0523	0.0000

2-3-4'-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2500	0.1250	0.0722	0.1667	0.2887	0.0625	0.0361	0.0208	0.0104	0.0208	0.0361	0.6019	0.3010	0.0125
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0722	0.0417	0.0208	0.0417	0.0722	0.3010	0.6019	0.0290
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1505	0.3010	0.0579
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.1158	0.1738	0.0334
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.3333	0.0833	0.0481	0.0278	0.0139	0.0278	0.0481	0.2006	0.1003	0.0167
6	0.2887	0.1443	0.0695	0.1925	0.3333	0.0000	0.0361	0.0241	0.0139	0.0069	0.0139	0.0241	0.3475	0.1738	0.0084
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.0752	0.1505	0.1003
8	0.0361	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0434	0.0869	0.2006
9	0.0208	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0251	0.0502	0.3475
10	0.0104	0.0208	0.0481	0.0278	0.0160	0.0093	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0125	0.0251	0.6019
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0251	0.0502	0.3475
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0434	0.0869	0.2006
13	0.6019	0.3010	0.1505	0.0869	0.2006	0.3475	0.0752	0.0434	0.0251	0.0125	0.0251	0.0434	0.0000	0.3623	0.0151
14	0.3010	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0869	0.0502	0.0251	0.0502	0.0869	0.3623	0.0000	0.0302
15	0.0125	0.0290	0.0579	0.0334	0.0193	0.0111	0.1158	0.2006	0.3475	0.6019	0.3475	0.2006	0.0151	0.0302	0.0000

2-4'-5-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.3333	0.0722	0.0417	0.0241	0.0120	0.0241	0.0417	0.3475	0.2006	0.0145
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1667	0.1250	0.0722	0.0417	0.0208	0.0417	0.0722	0.6019	0.0869	0.0251
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0833	0.2500	0.1443	0.0833	0.0417	0.0833	0.1443	0.3010	0.1738	0.0502
4	0.0962	0.1443	0.2887	0.0000	0.2887	0.1667	0.1443	0.0833	0.0481	0.0241	0.0481	0.0833	0.1738	0.3475	0.0290
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0481	0.0278	0.0120	0.0278	0.0481	0.1003	0.6019	0.0145
6	0.3333	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0241	0.0139	0.0069	0.0139	0.0241	0.2006	0.3475	0.0084
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0417	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.1505	0.0869	0.1003
8	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0869	0.0502	0.2006
9	0.0241	0.0417	0.0833	0.0481	0.0241	0.0139	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0502	0.0290	0.3475
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0069	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0251	0.0145	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0139	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0502	0.0290	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0869	0.0502	0.2006
13	0.3475	0.6019	0.3010	0.1738	0.0869	0.2006	0.1505	0.0869	0.0502	0.0251	0.0502	0.0869	0.0000	0.1046	0.0302
14	0.2006	0.1003	0.1738	0.3475	0.6019	0.3475	0.0869	0.0579	0.0334	0.0145	0.0334	0.0579	0.1208	0.0000	0.0174
15	0.0145	0.0251	0.0502	0.0290	0.0145	0.0084	0.1003	0.2006	0.3475	0.6019	0.3475	0.2006	0.0302	0.0174	0.0000

2-3-3'-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2500	0.1250	0.0722	0.1667	0.2887	0.0625	0.0361	0.0180	0.0104	0.0208	0.0361	0.6019	0.3010	0.0217
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0722	0.0361	0.0208	0.0417	0.0722	0.3010	0.6019	0.0434
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1443	0.0722	0.0417	0.0833	0.1443	0.1505	0.3010	0.0869
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0833	0.0417	0.0241	0.0481	0.0833	0.1158	0.1738	0.0502
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.3333	0.0833	0.0481	0.0241	0.0139	0.0278	0.0481	0.2006	0.1003	0.0290
6	0.2887	0.1443	0.0695	0.1925	0.3333	0.0000	0.0361	0.0208	0.0104	0.0060	0.0120	0.0208	0.3475	0.1738	0.0125
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2887	0.1443	0.0833	0.1667	0.2887	0.0752	0.1505	0.1738
8	0.0361	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.0000	0.2887	0.1667	0.0962	0.1667	0.0434	0.0869	0.3475
9	0.0180	0.0361	0.0722	0.0417	0.0241	0.0139	0.1443	0.2887	0.0000	0.2887	0.1667	0.0962	0.0217	0.0434	0.6019
10	0.0120	0.0241	0.0481	0.0278	0.0160	0.0093	0.0962	0.1667	0.2887	0.0000	0.3333	0.1925	0.0145	0.0290	0.3475
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.0962	0.1667	0.3333	0.0000	0.3333	0.0251	0.0502	0.2006
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1667	0.0833	0.1925	0.3333	0.0000	0.0434	0.0869	0.1003
13	0.6019	0.3010	0.1505	0.0869	0.2006	0.3475	0.0752	0.0434	0.0217	0.0125	0.0251	0.0434	0.0000	0.3623	0.0261
14	0.3010	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0869	0.0434	0.0251	0.0502	0.0869	0.3623	0.0000	0.0523
15	0.0217	0.0434	0.0869	0.0502	0.0290	0.0167	0.1738	0.3475	0.6019	0.3475	0.2006	0.1158	0.0261	0.0523	0.0000

3-4-4'-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2500	0.0722	0.0417	0.0241	0.0120	0.0241	0.0417	0.3010	0.6019	0.0145
2	0.2887	0.0000	0.2887	0.1667	0.0962	0.1443	0.1443	0.0833	0.0481	0.0241	0.0481	0.0833	0.1738	0.3475	0.0290
3	0.1443	0.2887	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0833	0.0417	0.0833	0.1443	0.1003	0.1738	0.0502
4	0.0833	0.1667	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0481	0.0241	0.0481	0.0833	0.2006	0.1003	0.0290
5	0.1443	0.0833	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0278	0.0139	0.0278	0.0481	0.3475	0.1738	0.0167
6	0.2500	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0208	0.0120	0.0060	0.0120	0.0208	0.6019	0.3010	0.0072
7	0.0722	0.1443	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.0502	0.0869	0.1003
8	0.0417	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0290	0.0502	0.2006
9	0.0241	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0167	0.0290	0.3475
10	0.0120	0.0241	0.0417	0.0241	0.0139	0.0069	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0084	0.0145	0.6019
11	0.0241	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0167	0.0290	0.3475
12	0.0417	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0290	0.0502	0.2006
13	0.3010	0.1738	0.0869	0.2006	0.3475	0.6019	0.0434	0.0251	0.0145	0.0072	0.0145	0.0251	0.0000	0.3623	0.0151
14	0.6019	0.3475	0.1738	0.1003	0.1738	0.3010	0.0869	0.0502	0.0290	0.0145	0.0290	0.0502	0.3623	0.0000	0.0174
15	0.0145	0.0290	0.0502	0.0290	0.0167	0.0084	0.1003	0.2006	0.3475	0.6019	0.3475	0.2006	0.0101	0.0174	0.0000

2-4-4'-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.2887	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.3475	0.3475	0.0167
2	0.2887	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.1738	0.6019	0.0290
3	0.1443	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1003	0.3010	0.0579
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.2006	0.1738	0.0334
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0278	0.0139	0.0278	0.0481	0.3475	0.1003	0.0167
6	0.2887	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0208	0.0120	0.0060	0.0417	0.0722	0.6019	0.1738	0.0072
7	0.0722	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.0502	0.1505	0.1003
8	0.0417	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0290	0.0869	0.2006
9	0.0241	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0167	0.0502	0.3475
10	0.0120	0.0208	0.0417	0.0241	0.0139	0.0069	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0084	0.0251	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0167	0.0502	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0290	0.0722	0.2006
13	0.3475	0.1738	0.0869	0.2006	0.3475	0.6019	0.0434	0.0251	0.0145	0.0072	0.0502	0.0869	0.0000	0.2092	0.0087
14	0.3475	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.2092	0.0000	0.0302
15	0.0145	0.0251	0.0502	0.0290	0.0167	0.0084	0.1003	0.2006	0.3475	0.6019	0.3475	0.2006	0.0101	0.0302	0.0000

2-4-5-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.1738	0.3475	0.3475
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.0869	0.1738	0.6019
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1738	0.0869	0.3010
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.3475	0.1738	0.1738
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0417	0.0241	0.0139	0.0120	0.0417	0.6019	0.3010	0.0869
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0208	0.0120	0.0069	0.0241	0.0208	0.3010	0.6019	0.1738
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.0869	0.0434	0.1505
8	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0502	0.0251	0.0869
9	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0290	0.0145	0.0502
10	0.0139	0.0241	0.0481	0.0278	0.0139	0.0069	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0167	0.0084	0.0290
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0290	0.0145	0.0502
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2500	0.1667	0.0962	0.1925	0.4013	0.0000	0.0502	0.0251	0.0869
13	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0502	0.0290	0.0167	0.0145	0.0502	0.0000	0.3623	0.1046
14	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0251	0.0145	0.0084	0.0290	0.0251	0.3623	0.0000	0.2092
15	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.1046	0.2092	0.0000

2-4-6-TRICHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.0869	0.3475	0.3475
2	0.2887	0.0000	0.2500	0.1250	0.0722	0.1443	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.1505	0.1738	0.6019
3	0.1443	0.2500	0.0000	0.2500	0.1443	0.0722	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.3010	0.0869	0.3010
4	0.0833	0.1250	0.2500	0.0000	0.2887	0.1443	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.6019	0.1738	0.1505
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.3475	0.3475	0.1003
6	0.2887	0.1443	0.0722	0.1443	0.2887	0.0000	0.0361	0.0208	0.0120	0.0069	0.0120	0.0208	0.1738	0.6019	0.1738
7	0.0722	0.1250	0.2500	0.1250	0.0722	0.0361	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.1505	0.0434	0.1505
8	0.0417	0.0722	0.1443	0.0722	0.0417	0.0241	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0869	0.0290	0.0869
9	0.0241	0.0417	0.0833	0.0417	0.0241	0.0120	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0502	0.0145	0.0502
10	0.0139	0.0241	0.0481	0.0241	0.0139	0.0069	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0290	0.0084	0.0290
11	0.0241	0.0417	0.0833	0.0417	0.0241	0.0120	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0502	0.0145	0.0502
12	0.0417	0.0722	0.1443	0.0722	0.0417	0.0241	0.2887	0.1667	0.0962	0.1925	0.4013	0.0000	0.0869	0.0290	0.0869
13	0.1003	0.1505	0.3010	0.6019	0.3475	0.1738	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.0000	0.2092	0.1812
14	0.3475	0.1738	0.0869	0.1738	0.3475	0.6019	0.0434	0.0251	0.0145	0.0084	0.0145	0.0251	0.2092	0.0000	0.2092
15	0.3475	0.6019	0.3010	0.1505	0.0869	0.1738	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.1812	0.2092	0.0000

2-2'-3-4-TETRA CHLORO BIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2500	0.1250	0.0722	0.1443	0.2500	0.0625	0.0313	0.0180	0.0104	0.0208	0.0361	0.3010	0.6019	0.3010	0.0376
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1250	0.1250	0.0625	0.0361	0.0208	0.0417	0.0722	0.1505	0.3010	0.6019	0.0752
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1250	0.0722	0.0417	0.0833	0.1443	0.1003	0.1505	0.3010	0.1505
4	0.0833	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0722	0.0417	0.0241	0.0481	0.0833	0.2006	0.1003	0.1738	0.0869
5	0.1443	0.0722	0.1667	0.3333	0.0000	0.2887	0.0833	0.0417	0.0241	0.0139	0.0278	0.0481	0.3475	0.1738	0.0869	0.0502
6	0.2500	0.1250	0.0625	0.1667	0.2887	0.0000	0.0313	0.0156	0.0120	0.0052	0.0104	0.0180	0.6019	0.3010	0.1505	0.0188
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2500	0.1443	0.0833	0.1667	0.2887	0.0502	0.0752	0.1505	0.3010
8	0.0313	0.0625	0.1250	0.0722	0.0417	0.0208	0.2500	0.0000	0.2887	0.1667	0.0962	0.1443	0.0251	0.0376	0.0752	0.6019
9	0.0180	0.0361	0.0722	0.0417	0.0241	0.0120	0.1443	0.2887	0.0000	0.3333	0.1925	0.1111	0.0145	0.0217	0.0434	0.3475
10	0.0120	0.0241	0.0481	0.0278	0.0160	0.0080	0.0962	0.1667	0.3333	0.0000	0.3333	0.1925	0.0097	0.0145	0.0290	0.2006
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0833	0.1925	0.3333	0.0000	0.3333	0.0167	0.0251	0.0502	0.1003
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1443	0.0833	0.1925	0.3333	0.0000	0.0290	0.0434	0.0869	0.1738
13	0.3010	0.1505	0.0752	0.2006	0.3475	0.6019	0.0376	0.0188	0.0145	0.0063	0.0125	0.0217	0.0000	0.3623	0.1812	0.0226
14	0.6019	0.3010	0.1505	0.0869	0.1738	0.3010	0.0752	0.0376	0.0217	0.0125	0.0251	0.0434	0.3623	0.0000	0.3623	0.0453
15	0.3010	0.6019	0.3010	0.1738	0.1003	0.1505	0.1505	0.0752	0.0434	0.0251	0.0502	0.0869	0.1812	0.3623	0.0000	0.0906
16	0.0376	0.0752	0.1505	0.0869	0.0502	0.0251	0.3010	0.6019	0.3475	0.2006	0.1158	0.1738	0.0302	0.0453	0.0906	0.0000

2-2'-3-5'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2500	0.1250	0.0722	0.1667	0.2887	0.0625	0.0313	0.0180	0.0104	0.0180	0.0361	0.6019	0.3010	0.0376	0.0217
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.3010	0.6019	0.0752	0.0434
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1250	0.0722	0.0417	0.0722	0.1443	0.1505	0.3010	0.1505	0.0869
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0722	0.0417	0.0241	0.0417	0.0833	0.1158	0.1738	0.0869	0.0502
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.3333	0.0833	0.0417	0.0241	0.0139	0.0241	0.0481	0.2006	0.1003	0.0502	0.0290
6	0.2887	0.1443	0.0722	0.1925	0.3333	0.0000	0.0361	0.0180	0.0104	0.0060	0.0104	0.0208	0.3475	0.1738	0.0217	0.0125
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2500	0.1443	0.0833	0.1443	0.2887	0.0752	0.1505	0.3010	0.1738
8	0.0313	0.0625	0.1250	0.0722	0.0417	0.0241	0.2500	0.0000	0.2887	0.1667	0.0833	0.1443	0.0376	0.0752	0.6019	0.1003
9	0.0180	0.0361	0.0722	0.0417	0.0241	0.0139	0.1443	0.2887	0.0000	0.3333	0.1667	0.0962	0.0217	0.0434	0.3475	0.2006
10	0.0104	0.0208	0.0417	0.0241	0.0139	0.0080	0.0833	0.1667	0.3333	0.0000	0.2887	0.1667	0.0125	0.0251	0.2006	0.3475
11	0.0180	0.0361	0.0722	0.0417	0.0241	0.0139	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0217	0.0434	0.0869	0.6019
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1443	0.0833	0.1667	0.2887	0.0000	0.0434	0.0869	0.1738	0.3475
13	0.6019	0.3010	0.1505	0.0869	0.2006	0.3475	0.0752	0.0376	0.0217	0.0125	0.0217	0.0434	0.0000	0.3623	0.0453	0.0261
14	0.3010	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.3623	0.0000	0.0906	0.0523
15	0.0376	0.0752	0.1505	0.0869	0.0502	0.0290	0.3010	0.6019	0.3475	0.2006	0.1003	0.1738	0.0453	0.0906	0.0000	0.1208
16	0.0217	0.0434	0.0869	0.0502	0.0290	0.0167	0.1738	0.0869	0.2006	0.3475	0.6019	0.3475	0.0261	0.0523	0.1046	0.0000

2-2'-4-4'- TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.2887	0.0722	0.0361	0.0208	0.0104	0.0241	0.0417	0.3475	0.3475	0.0434	0.0125
2	0.2887	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0625	0.0361	0.0180	0.0417	0.0722	0.1738	0.6019	0.0752	0.0217
3	0.1443	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1250	0.0722	0.0361	0.0833	0.1443	0.1003	0.3010	0.1505	0.0434
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0722	0.0417	0.0208	0.0481	0.0833	0.2006	0.1738	0.0869	0.0251
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.2887	0.0833	0.0417	0.0241	0.0120	0.0278	0.0481	0.3475	0.1003	0.0502	0.0145
6	0.2887	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0180	0.0090	0.0052	0.0120	0.0208	0.6019	0.1738	0.0217	0.0063
7	0.0722	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2500	0.1443	0.0722	0.1667	0.2887	0.0502	0.1505	0.3010	0.0869
8	0.0361	0.0625	0.1250	0.0722	0.0417	0.0208	0.2500	0.0000	0.2887	0.1443	0.0962	0.1443	0.0251	0.0752	0.6019	0.1738
9	0.0208	0.0361	0.0722	0.0417	0.0241	0.0120	0.1443	0.2887	0.0000	0.2887	0.1925	0.1111	0.0145	0.0434	0.3475	0.3475
10	0.0120	0.0208	0.0417	0.0241	0.0139	0.0069	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.0084	0.0251	0.1738	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0833	0.1925	0.2887	0.0000	0.3333	0.0167	0.0502	0.1003	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1443	0.0833	0.1667	0.3333	0.0000	0.0290	0.0869	0.1738	0.2006
13	0.3475	0.1738	0.0869	0.2006	0.3475	0.6019	0.0434	0.0217	0.0109	0.0063	0.0145	0.0251	0.0000	0.2092	0.0261	0.0075
14	0.3475	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0752	0.0434	0.0217	0.0502	0.0869	0.2092	0.0000	0.0906	0.0261
15	0.0434	0.0752	0.1505	0.0869	0.0502	0.0251	0.3010	0.6019	0.3475	0.1738	0.1158	0.1738	0.0302	0.0906	0.0000	0.2092
16	0.0145	0.0251	0.0502	0.0290	0.0167	0.0084	0.1003	0.1738	0.3475	0.6019	0.3475	0.2006	0.0101	0.0302	0.2092	0.0000

2-3-4-4'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2500	0.1250	0.0722	0.1443	0.2500	0.0625	0.0361	0.0208	0.0104	0.0208	0.0361	0.3010	0.6019	0.3010	0.0125
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1250	0.1250	0.0722	0.0417	0.0208	0.0417	0.0722	0.1505	0.3010	0.6019	0.0251
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0833	0.0417	0.0833	0.1443	0.1003	0.1505	0.3010	0.0502
4	0.0833	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0481	0.0241	0.0481	0.0833	0.2006	0.1003	0.1738	0.0290
5	0.1443	0.0722	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0278	0.0139	0.0278	0.0481	0.3475	0.1738	0.0869	0.0167
6	0.2500	0.1250	0.0625	0.1667	0.2887	0.0000	0.0313	0.0180	0.0104	0.0052	0.0104	0.0180	0.6019	0.3010	0.1505	0.0063
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.0502	0.0752	0.1505	0.1003
8	0.0361	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0290	0.0434	0.0869	0.2006
9	0.0208	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0167	0.0251	0.0502	0.3475
10	0.0104	0.0208	0.0417	0.0241	0.0160	0.0069	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0084	0.0125	0.0251	0.6019
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0167	0.0251	0.0502	0.3475
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0290	0.0434	0.0869	0.2006
13	0.3010	0.1505	0.0752	0.2006	0.3475	0.6019	0.0376	0.0217	0.0125	0.0063	0.0125	0.0217	0.0000	0.3623	0.1812	0.0075
14	0.6019	0.3010	0.1505	0.0869	0.1738	0.3010	0.0752	0.0434	0.0251	0.0125	0.0251	0.0434	0.3623	0.0000	0.3623	0.0151
15	0.3010	0.6019	0.3010	0.1738	0.1003	0.1505	0.1505	0.0869	0.0502	0.0251	0.0502	0.0869	0.1812	0.3623	0.0000	0.0302
16	0.0125	0.0251	0.0502	0.0290	0.0193	0.0084	0.1003	0.2006	0.3475	0.6019	0.3475	0.2006	0.0101	0.0151	0.0302	0.0000

2-2'-5-5'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.3333	0.0722	0.0361	0.0208	0.0120	0.0208	0.0417	0.3475	0.0434	0.2006	0.0251
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1667	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.6019	0.0752	0.0869	0.0434
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0833	0.2500	0.1250	0.0722	0.0417	0.0722	0.1443	0.3010	0.1505	0.1738	0.0869
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.1443	0.0722	0.0417	0.0241	0.0417	0.0833	0.1738	0.0869	0.3475	0.0502
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0208	0.0120	0.0208	0.0417	0.1003	0.0434	0.6019	0.0251
6	0.3333	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0208	0.0120	0.0069	0.0120	0.0241	0.2006	0.0251	0.3475	0.0145
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0417	0.0000	0.2500	0.1443	0.0833	0.1443	0.2887	0.1505	0.3010	0.0869	0.1738
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0208	0.2500	0.0000	0.2887	0.1667	0.0833	0.1443	0.0752	0.6019	0.0434	0.1003
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0120	0.1443	0.2887	0.0000	0.3333	0.1667	0.0962	0.0434	0.3475	0.0251	0.2006
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0069	0.0833	0.1667	0.3333	0.0000	0.2887	0.1667	0.0251	0.2006	0.0145	0.3475
11	0.0208	0.0361	0.0722	0.0417	0.0208	0.0120	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0434	0.0869	0.0251	0.6019
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.1443	0.0833	0.1667	0.2887	0.0000	0.0869	0.1738	0.0502	0.3475
13	0.3475	0.6019	0.3010	0.1738	0.0869	0.2006	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.0000	0.0906	0.1046	0.0523
14	0.0434	0.0752	0.1505	0.0869	0.0434	0.0251	0.3010	0.6019	0.3475	0.2006	0.1003	0.1738	0.0906	0.0000	0.0523	0.1208
15	0.2006	0.1003	0.1738	0.3475	0.6019	0.3475	0.0869	0.0434	0.0251	0.0145	0.0251	0.0502	0.1208	0.0523	0.0000	0.0302
16	0.0251	0.0434	0.0869	0.0502	0.0251	0.0145	0.1738	0.0869	0.2006	0.3475	0.6019	0.3475	0.0523	0.1046	0.0302	0.0000

2-3'-4-4'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.2887	0.0722	0.0417	0.0208	0.0104	0.0241	0.0417	0.3475	0.3475	0.0251	0.0125
2	0.2887	0.0000	0.2500	0.1443	0.0833	0.0722	0.1250	0.0722	0.0361	0.0180	0.0417	0.0722	0.0869	0.6019	0.0434	0.0217
3	0.1443	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0722	0.0361	0.0833	0.1443	0.1003	0.3010	0.0869	0.0434
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0417	0.0208	0.0481	0.0833	0.2006	0.1738	0.0502	0.0251
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0241	0.0120	0.0278	0.0481	0.3475	0.1003	0.0290	0.0145
6	0.2887	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0208	0.0104	0.0052	0.0120	0.0208	0.6019	0.1738	0.0125	0.0063
7	0.0722	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.0502	0.1505	0.1738	0.0869
8	0.0417	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.2887	0.1443	0.0833	0.1667	0.0290	0.0869	0.3475	0.1738
9	0.0208	0.0361	0.0722	0.0417	0.0241	0.0120	0.1443	0.2887	0.0000	0.2500	0.1443	0.0833	0.0145	0.0434	0.6019	0.3010
10	0.0120	0.0208	0.0417	0.0241	0.0139	0.0069	0.0833	0.1443	0.2500	0.0000	0.2887	0.1667	0.0084	0.0251	0.3010	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1443	0.2887	0.0000	0.3333	0.0167	0.0502	0.1738	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0833	0.1667	0.3333	0.0000	0.0290	0.0869	0.1003	0.2006
13	0.3475	0.1738	0.0869	0.2006	0.3475	0.6019	0.0434	0.0251	0.0125	0.0063	0.0145	0.0251	0.0000	0.2092	0.0151	0.0075
14	0.3475	0.6019	0.3010	0.1738	0.1003	0.0869	0.1505	0.0869	0.0434	0.0217	0.0502	0.0869	0.2092	0.0000	0.0523	0.0261
15	0.0251	0.0434	0.0869	0.0502	0.0290	0.0145	0.1738	0.3475	0.6019	0.3010	0.1738	0.1003	0.0174	0.0523	0.0000	0.3623
16	0.0145	0.0251	0.0502	0.0290	0.0167	0.0084	0.1003	0.1738	0.3010	0.6019	0.3475	0.2006	0.0101	0.0302	0.3623	0.0000

2-3'-4'-5-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.3333	0.0722	0.0417	0.0208	0.0104	0.0241	0.0417	0.2006	0.3475	0.0251	0.0125
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1667	0.1250	0.0722	0.0361	0.0180	0.0417	0.0722	0.0869	0.6019	0.0434	0.0217
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0833	0.2500	0.1443	0.0722	0.0361	0.0833	0.1443	0.1738	0.3010	0.0869	0.0434
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.1443	0.0833	0.0417	0.0208	0.0481	0.0833	0.3475	0.1738	0.0502	0.0251
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0417	0.0208	0.0104	0.0241	0.0417	0.6019	0.1003	0.0251	0.0125
6	0.3333	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0241	0.0120	0.0104	0.0139	0.0241	0.3475	0.2006	0.0145	0.0125
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0417	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.0869	0.1505	0.1738	0.0869
8	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.0000	0.2887	0.1443	0.0833	0.1667	0.0502	0.0869	0.3475	0.1738
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0120	0.1443	0.2887	0.0000	0.2500	0.1443	0.0833	0.0251	0.0434	0.6019	0.3010
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0069	0.0833	0.1443	0.2500	0.0000	0.2887	0.1667	0.0145	0.0251	0.3010	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0139	0.1667	0.0962	0.1443	0.2887	0.0000	0.3333	0.0290	0.0502	0.1738	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.1667	0.0833	0.1667	0.3333	0.0000	0.0502	0.0869	0.1003	0.2006
13	0.2006	0.1003	0.1738	0.3475	0.6019	0.3475	0.0869	0.0502	0.0251	0.0125	0.0290	0.0502	0.0000	0.1208	0.0302	0.0151
14	0.3475	0.6019	0.3010	0.1738	0.0869	0.2006	0.1505	0.0869	0.0434	0.0217	0.0502	0.0869	0.1046	0.0000	0.0523	0.0261
15	0.0251	0.0434	0.0869	0.0502	0.0251	0.0145	0.1738	0.3475	0.6019	0.3010	0.1738	0.1003	0.0302	0.0523	0.0000	0.3623
16	0.0145	0.0251	0.0502	0.0290	0.0145	0.0084	0.1003	0.1738	0.3010	0.6019	0.3475	0.2006	0.0174	0.0302	0.3623	0.0000

2-2'-3-3'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2500	0.1250	0.0722	0.1667	0.2887	0.0625	0.0313	0.0156	0.0090	0.0208	0.0361	0.6019	0.3010	0.0376	0.0188
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1443	0.1250	0.0625	0.0313	0.0180	0.0417	0.0722	0.3010	0.6019	0.0752	0.0376
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0962	0.2500	0.1250	0.0625	0.0361	0.0833	0.1443	0.1505	0.3010	0.1505	0.0752
4	0.0962	0.1443	0.2887	0.0000	0.3333	0.1925	0.1443	0.0722	0.0361	0.0208	0.0481	0.0833	0.1158	0.1738	0.0869	0.0434
5	0.1667	0.0833	0.1667	0.3333	0.0000	0.3333	0.0833	0.0417	0.0208	0.0120	0.0278	0.0481	0.2006	0.1003	0.0502	0.0251
6	0.2887	0.1443	0.0722	0.1925	0.3333	0.0000	0.0361	0.0180	0.0090	0.0052	0.0054	0.0208	0.3475	0.1738	0.0217	0.0109
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0481	0.0000	0.2500	0.1250	0.0722	0.1667	0.2887	0.0752	0.1505	0.3010	0.1505
8	0.0313	0.0625	0.1250	0.0722	0.0417	0.0241	0.2500	0.0000	0.2500	0.1443	0.0833	0.1443	0.0376	0.0752	0.6019	0.3010
9	0.0156	0.0313	0.0625	0.0361	0.0208	0.0120	0.1250	0.2500	0.0000	0.2887	0.1667	0.0962	0.0188	0.0376	0.3010	0.6019
10	0.0120	0.0241	0.0481	0.0278	0.0160	0.0093	0.0962	0.1443	0.2887	0.0000	0.3333	0.1925	0.0145	0.0290	0.1738	0.3475
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0160	0.1667	0.0833	0.1667	0.3333	0.0000	0.3333	0.0251	0.0502	0.1003	0.2006
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0278	0.2887	0.1443	0.0722	0.1925	0.3333	0.0000	0.0434	0.0869	0.1738	0.0869
13	0.6019	0.3010	0.1505	0.0869	0.2006	0.3475	0.0752	0.0376	0.0188	0.0109	0.0251	0.0434	0.0000	0.3623	0.0453	0.0226
14	0.3010	0.6019	0.3010	0.1738	0.1003	0.1738	0.1505	0.0752	0.0376	0.0217	0.0502	0.0869	0.3623	0.0000	0.0906	0.0453
15	0.0376	0.0752	0.1505	0.0869	0.0502	0.0290	0.3010	0.6019	0.3010	0.1738	0.1003	0.1738	0.0453	0.0906	0.0000	0.3623
16	0.0188	0.0376	0.0752	0.0434	0.0251	0.0145	0.1505	0.3010	0.6019	0.3475	0.2006	0.1158	0.0226	0.0453	0.3623	0.0000

2-2'-6-6'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0722	0.1925	0.3333	0.0722	0.0361	0.0208	0.0120	0.0208	0.0361	0.3475	0.0434	0.0869	0.0434
2	0.2887	0.0000	0.2500	0.1250	0.0722	0.1667	0.0722	0.0625	0.0361	0.0208	0.0361	0.0625	0.6019	0.0752	0.1505	0.0752
3	0.1443	0.2500	0.0000	0.2500	0.1443	0.0833	0.2500	0.1250	0.0722	0.0417	0.0722	0.1250	0.3010	0.1505	0.3010	0.1505
4	0.0962	0.1250	0.2500	0.0000	0.2887	0.1667	0.1250	0.0625	0.0361	0.0208	0.0361	0.0625	0.1505	0.0752	0.6019	0.0752
5	0.1925	0.0962	0.1443	0.2887	0.0000	0.3333	0.0722	0.0361	0.0208	0.0120	0.0208	0.0361	0.1158	0.0434	0.3475	0.0434
6	0.3333	0.1667	0.0833	0.1667	0.3333	0.0000	0.0417	0.0208	0.0120	0.0069	0.0120	0.0208	0.2006	0.0251	0.2006	0.0251
7	0.0722	0.1250	0.2500	0.1250	0.0722	0.0417	0.0000	0.2500	0.1443	0.0833	0.1443	0.2500	0.1505	0.3010	0.1505	0.3010
8	0.0361	0.0625	0.1250	0.2500	0.0361	0.0208	0.2500	0.0000	0.2887	0.1667	0.0962	0.1250	0.0752	0.6019	0.3010	0.1505
9	0.0208	0.0361	0.0722	0.0361	0.0208	0.0120	0.1443	0.2887	0.0000	0.3333	0.1925	0.0962	0.0434	0.3475	0.0434	0.1158
10	0.0120	0.0208	0.0417	0.0208	0.0120	0.0069	0.0833	0.1667	0.3333	0.0000	0.3333	0.2887	0.0251	0.2006	0.0251	0.2006
11	0.0208	0.0361	0.0722	0.0361	0.0208	0.0120	0.1443	0.0722	0.1925	0.3333	0.0000	0.1667	0.0434	0.0869	0.0434	0.3475
12	0.0361	0.0625	0.1250	0.0625	0.0361	0.0208	0.2500	0.1250	0.0722	0.1667	0.2887	0.0000	0.0752	0.1505	0.0752	0.6019
13	0.3475	0.6019	0.3010	0.1505	0.0869	0.2006	0.0869	0.0752	0.0434	0.0251	0.0434	0.0752	0.0000	0.0906	0.1812	0.0906
14	0.0434	0.0752	0.1505	0.3010	0.0434	0.0251	0.3010	0.6019	0.3475	0.2006	0.1158	0.1505	0.0906	0.0000	0.3623	0.1812
15	0.1158	0.1505	0.3010	0.6019	0.3475	0.2006	0.1505	0.0752	0.0434	0.0251	0.0434	0.0752	0.1812	0.0906	0.0000	0.0906
16	0.0434	0.0752	0.1505	0.0752	0.0434	0.0251	0.3010	0.1505	0.0869	0.2006	0.3475	0.6019	0.0906	0.1812	0.0906	0.0000

3-3'-4-4'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2500	0.0722	0.0417	0.0208	0.0104	0.0241	0.0417	0.3010	0.6019	0.0251	0.0125
2	0.2887	0.0000	0.2887	0.1667	0.0962	0.1443	0.1443	0.0833	0.0417	0.0208	0.0481	0.0833	0.1738	0.3475	0.0502	0.0251
3	0.1443	0.2887	0.0000	0.2887	0.1667	0.0833	0.2500	0.1443	0.0722	0.0361	0.0833	0.1443	0.1003	0.1738	0.0869	0.0434
4	0.0833	0.1667	0.2887	0.0000	0.3333	0.1667	0.1443	0.0833	0.0417	0.0208	0.0481	0.0833	0.2006	0.1003	0.0502	0.0251
5	0.1443	0.0833	0.1667	0.3333	0.0000	0.2887	0.0833	0.0481	0.0241	0.0120	0.0278	0.0481	0.3475	0.1738	0.0290	0.0145
6	0.2500	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0208	0.0104	0.0052	0.0120	0.0208	0.6019	0.3010	0.0125	0.0063
7	0.0722	0.1443	0.2500	0.1443	0.0833	0.0417	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.0502	0.0869	0.1738	0.0869
8	0.0417	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.0000	0.2887	0.1443	0.0833	0.1667	0.0290	0.0502	0.3475	0.1738
9	0.0208	0.0417	0.0722	0.0417	0.0241	0.0120	0.1443	0.2887	0.0000	0.2500	0.1443	0.0833	0.0145	0.0251	0.6019	0.3010
10	0.0120	0.0241	0.0417	0.0241	0.0139	0.0069	0.0833	0.1443	0.2500	0.0000	0.2887	0.1667	0.0084	0.0145	0.3010	0.6019
11	0.0241	0.0481	0.0833	0.0481	0.0278	0.0139	0.1667	0.0962	0.1443	0.2887	0.0000	0.3333	0.0167	0.0290	0.1738	0.3475
12	0.0417	0.0833	0.1443	0.0833	0.0481	0.0241	0.2887	0.1667	0.0833	0.1667	0.3333	0.0000	0.0290	0.0502	0.1003	0.2006
13	0.3010	0.1738	0.0869	0.2006	0.3475	0.6019	0.0434	0.0251	0.0125	0.0063	0.0145	0.0251	0.0000	0.3623	0.0151	0.0075
14	0.6019	0.3475	0.1738	0.1003	0.1738	0.3010	0.0869	0.0502	0.0251	0.0125	0.0290	0.0502	0.3623	0.0000	0.0302	0.0151
15	0.0251	0.0502	0.0869	0.0502	0.0290	0.0145	0.1738	0.3475	0.6019	0.3010	0.1738	0.1003	0.0174	0.0302	0.0000	0.3623
16	0.0145	0.0290	0.0502	0.0290	0.0167	0.0084	0.1003	0.1738	0.3010	0.6019	0.3475	0.2006	0.0101	0.0174	0.3623	0.0000

2-3-5-6-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2500	0.1250	0.0625	0.1443	0.2887	0.0625	0.0361	0.0208	0.0120	0.0208	0.0361	0.6019	0.3010	0.1738	0.0752
2	0.2500	0.0000	0.2500	0.1250	0.0625	0.1443	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.3010	0.6019	0.0752	0.1505
3	0.1250	0.2500	0.0000	0.2500	0.1250	0.0722	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1505	0.3010	0.1505	0.3010
4	0.0722	0.1250	0.2500	0.0000	0.2500	0.1443	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.0869	0.1505	0.3010	0.6019
5	0.1443	0.0722	0.1250	0.2500	0.0000	0.2887	0.0625	0.0361	0.0208	0.0120	0.0208	0.0361	0.1738	0.0869	0.6019	0.3010
6	0.2887	0.1443	0.0722	0.1443	0.2887	0.0000	0.0361	0.0208	0.0120	0.0069	0.1667	0.0208	0.3475	0.1738	0.3475	0.1738
7	0.0625	0.1250	0.2500	0.1250	0.0625	0.0361	0.0000	0.2887	0.1667	0.0962	0.0120	0.2887	0.0752	0.1505	0.0752	0.1505
8	0.0361	0.0722	0.1443	0.0722	0.0361	0.0208	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0434	0.0869	0.0434	0.0869
9	0.0208	0.0417	0.0833	0.0417	0.0208	0.0120	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0251	0.0502	0.0251	0.0502
10	0.0120	0.0241	0.0481	0.0241	0.0120	0.0069	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0145	0.0290	0.0145	0.0290
11	0.0208	0.0417	0.0833	0.0417	0.0208	0.0120	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0251	0.0502	0.0251	0.0502
12	0.0361	0.0722	0.1443	0.0722	0.0361	0.0208	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0434	0.0869	0.0434	0.0869
13	0.6019	0.3010	0.1505	0.0752	0.1738	0.3475	0.0752	0.0434	0.0251	0.0145	0.0251	0.0434	0.0000	0.3623	0.2092	0.0906
14	0.3010	0.6019	0.3010	0.1505	0.0752	0.1738	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.3623	0.0000	0.0906	0.1812
15	0.1738	0.0869	0.1505	0.3010	0.6019	0.3475	0.0752	0.0434	0.0251	0.0145	0.0251	0.0434	0.2092	0.1046	0.0000	0.3623
16	0.0869	0.1505	0.3010	0.6019	0.3010	0.1738	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.1046	0.1812	0.3623	0.0000

2-4-4'-5-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0417	0.0241	0.0120	0.0241	0.0417	0.3475	0.3475	0.1738	0.0145
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0722	0.0417	0.0208	0.0417	0.0722	0.1738	0.6019	0.0869	0.0251
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1443	0.0833	0.0417	0.0833	0.1443	0.0869	0.3010	0.1738	0.0502
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0833	0.0481	0.0241	0.0481	0.0833	0.1738	0.1738	0.3475	0.0290
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0417	0.0241	0.0120	0.0241	0.0417	0.3010	0.0869	0.6019	0.0145
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0208	0.0120	0.0060	0.0139	0.0208	0.6019	0.1738	0.3010	0.0072
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2887	0.1667	0.0833	0.1667	0.2887	0.0434	0.1505	0.0869	0.1003
8	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.0000	0.3333	0.1667	0.0962	0.1667	0.0251	0.0869	0.0502	0.2006
9	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.3333	0.0000	0.2887	0.1667	0.0962	0.0145	0.0502	0.0290	0.3475
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0060	0.0833	0.1667	0.2887	0.0000	0.2887	0.1667	0.0072	0.0251	0.0145	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0962	0.1667	0.2887	0.0000	0.3333	0.0145	0.0502	0.0290	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1667	0.0962	0.1667	0.3333	0.0000	0.0251	0.0869	0.0502	0.2006
13	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0251	0.0145	0.0072	0.0167	0.0251	0.0000	0.2092	0.3623	0.0087
14	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0869	0.0502	0.0251	0.0502	0.0869	0.2092	0.0000	0.1046	0.0302
15	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0502	0.0290	0.0145	0.0290	0.0502	0.3623	0.1046	0.0000	0.0174
16	0.0145	0.0251	0.0502	0.0290	0.0145	0.0072	0.1003	0.2006	0.3475	0.6019	0.3475	0.2006	0.0087	0.0302	0.0174	0.0000

2-3-4-5-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2500	0.1250	0.0722	0.1250	0.2500	0.0625	0.0361	0.0208	0.0120	0.0208	0.0361	0.1505	0.3010	0.6019	0.3010
2	0.2500	0.0000	0.2500	0.1443	0.0722	0.1250	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.0869	0.1505	0.3010	0.6019
3	0.1250	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.1738	0.0869	0.1505	0.3010
4	0.0722	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0833	0.0481	0.0278	0.0481	0.0833	0.3475	0.1738	0.0869	0.1738
5	0.1250	0.0625	0.1443	0.2887	0.0000	0.2500	0.0722	0.0417	0.0241	0.0139	0.0241	0.0417	0.6019	0.3010	0.1505	0.0752
6	0.2500	0.1250	0.0625	0.1443	0.2500	0.0000	0.0313	0.0180	0.0104	0.0060	0.0104	0.0180	0.3010	0.6019	0.3010	0.1505
7	0.0625	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.0869	0.0434	0.0752	0.1505
8	0.0361	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.0000	0.3333	0.1925	0.1111	0.1667	0.0502	0.0251	0.0434	0.0869
9	0.0208	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0290	0.0145	0.0251	0.0502
10	0.0120	0.0241	0.0481	0.0278	0.0139	0.0069	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0167	0.0084	0.0145	0.0290
11	0.0208	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0290	0.0145	0.0251	0.0502
12	0.0361	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0502	0.0251	0.0434	0.0869
13	0.1505	0.0752	0.1738	0.3475	0.6019	0.3010	0.0869	0.0502	0.0290	0.0167	0.0290	0.0502	0.0000	0.3623	0.1812	0.0906
14	0.3010	0.1505	0.0752	0.1738	0.3010	0.6019	0.0376	0.0217	0.0125	0.0072	0.0125	0.0217	0.3623	0.0000	0.3623	0.1812
15	0.6019	0.3010	0.1505	0.0869	0.1505	0.3010	0.0752	0.0434	0.0251	0.0145	0.0251	0.0434	0.1812	0.3623	0.0000	0.3623
16	0.3010	0.6019	0.3010	0.1738	0.0869	0.1505	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.1046	0.1812	0.3623	0.0000

2-2'-4-5-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0361	0.0208	0.0120	0.0241	0.0417	0.1738	0.3475	0.3475	0.0434
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0625	0.0361	0.0208	0.0417	0.0722	0.0869	0.1738	0.6019	0.0752
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0722	0.0417	0.0833	0.1443	0.1738	0.0869	0.3010	0.1505
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0417	0.0241	0.0481	0.0833	0.3475	0.1738	0.1738	0.0869
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0208	0.0120	0.0241	0.0417	0.6019	0.3010	0.0869	0.0434
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0180	0.0104	0.0060	0.0120	0.0208	0.3010	0.6019	0.1738	0.0217
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1443	0.0833	0.1667	0.2887	0.0869	0.0434	0.1505	0.3010
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2887	0.1667	0.0962	0.1443	0.0434	0.0217	0.0752	0.6019
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.3333	0.1925	0.1111	0.0251	0.0125	0.0434	0.3475
10	0.0139	0.0241	0.0481	0.0278	0.0139	0.0069	0.0962	0.1667	0.3333	0.0000	0.3333	0.1925	0.0167	0.0084	0.0290	0.2006
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0833	0.1925	0.3333	0.0000	0.3333	0.0290	0.0145	0.0502	0.1003
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0833	0.1925	0.3333	0.0000	0.0502	0.0251	0.0869	0.1738
13	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0251	0.0145	0.0290	0.0502	0.0000	0.3623	0.1046	0.0523
14	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0217	0.0125	0.0072	0.0145	0.0251	0.3623	0.0000	0.2092	0.0261
15	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0752	0.0434	0.0251	0.0502	0.0869	0.1046	0.2092	0.0000	0.0906
16	0.0434	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3475	0.2006	0.1158	0.1738	0.0523	0.0261	0.0906	0.0000

2-2'-5-6'-TETRACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.2887	0.1443	0.0833	0.1667	0.3333	0.0722	0.0361	0.0208	0.0120	0.0208	0.0361	0.2006	0.3475	0.0434	0.0434
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1667	0.1250	0.0625	0.0361	0.0208	0.0361	0.0625	0.0869	0.6019	0.0752	0.0752
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0833	0.2500	0.1250	0.0722	0.0417	0.0722	0.1250	0.1738	0.3010	0.1505	0.1505
4	0.0962	0.1443	0.2887	0.0000	0.2887	0.1667	0.1443	0.0722	0.0417	0.0241	0.0417	0.0722	0.3475	0.1738	0.0869	0.0869
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0208	0.0120	0.0208	0.0361	0.6019	0.1003	0.0434	0.0434
6	0.3333	0.1667	0.0833	0.1667	0.2887	0.0000	0.0417	0.0208	0.0120	0.0069	0.0120	0.0208	0.3475	0.2006	0.0251	0.0251
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0417	0.0000	0.2500	0.0722	0.0833	0.1443	0.2500	0.0869	0.1505	0.3010	0.3010
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0208	0.2500	0.0000	0.2887	0.1667	0.0962	0.1250	0.0434	0.0752	0.6019	0.1505
9	0.0208	0.0361	0.0722	0.0417	0.0361	0.0120	0.1443	0.2887	0.0000	0.3333	0.1925	0.0962	0.0434	0.0434	0.3475	0.1158
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0069	0.0833	0.1667	0.3333	0.0000	0.3333	0.1667	0.0145	0.0251	0.2006	0.2006
11	0.0208	0.0361	0.0722	0.0417	0.0361	0.0120	0.1443	0.0722	0.1925	0.3333	0.0000	0.2887	0.0434	0.0434	0.0869	0.3475
12	0.0361	0.0625	0.1250	0.0722	0.0361	0.0208	0.2500	0.1250	0.0722	0.1667	0.2887	0.0000	0.0434	0.0752	0.1505	0.6019
13	0.2006	0.1003	0.1738	0.3475	0.6019	0.3475	0.0869	0.0434	0.0251	0.0145	0.0251	0.0434	0.0000	0.1208	0.0523	0.0523
14	0.3475	0.6019	0.3010	0.1738	0.0869	0.2006	0.1505	0.0752	0.0434	0.0251	0.0434	0.0752	0.1046	0.0000	0.0906	0.0906
15	0.0434	0.0752	0.1505	0.0869	0.0434	0.0251	0.3010	0.6019	0.3475	0.2006	0.1158	0.1505	0.0523	0.0906	0.0000	0.1812
16	0.0434	0.0752	0.1505	0.0869	0.0434	0.0251	0.3010	0.1505	0.0869	0.2006	0.3475	0.6019	0.0523	0.0906	0.1812	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2500	0.1250	0.0625	0.1250	0.2500	0.0625	0.0361	0.0208	0.0120	0.0208	0.0361	0.0752	0.1505	0.3010	0.6019	0.3010
2	0.2500	0.0000	0.2500	0.1250	0.0625	0.1250	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.1505	0.0752	0.1505	0.3010	0.6019
3	0.1250	0.2500	0.0000	0.2500	0.1250	0.0625	0.2500	0.1443	0.0833	0.0481	0.0833	0.1443	0.3010	0.1505	0.0752	0.1505	0.3010
4	0.0625	0.1250	0.2500	0.0000	0.2500	0.1250	0.1250	0.0722	0.0417	0.0241	0.0417	0.0722	0.6019	0.3010	0.1505	0.0752	0.1505
5	0.1250	0.0625	0.1250	0.2500	0.0000	0.2500	0.0625	0.0361	0.0208	0.0120	0.0208	0.0361	0.3010	0.6019	0.3010	0.1505	0.0752
6	0.2500	0.1250	0.0625	0.1250	0.2500	0.0000	0.0313	0.0180	0.0104	0.0060	0.0104	0.0180	0.1505	0.3010	0.6019	0.3010	0.1505
7	0.0625	0.1250	0.2500	0.1250	0.0625	0.0313	0.0000	0.2887	0.1667	0.0962	0.1667	0.2887	0.1505	0.0752	0.0376	0.0752	0.1505
8	0.0361	0.0722	0.1443	0.0722	0.0361	0.0180	0.2887	0.0000	0.3333	0.1925	0.3333	0.1667	0.0869	0.0434	0.0217	0.0434	0.0869
9	0.0208	0.0417	0.0833	0.0417	0.0208	0.0104	0.1667	0.3333	0.0000	0.3333	0.1925	0.1111	0.0502	0.0251	0.0125	0.0251	0.0502
10	0.0120	0.0241	0.0481	0.0241	0.0120	0.0060	0.0962	0.1925	0.3333	0.0000	0.3333	0.1925	0.0290	0.0145	0.0072	0.0145	0.0290
11	0.0208	0.0417	0.0833	0.0417	0.0208	0.0104	0.1667	0.0962	0.1925	0.3333	0.0000	0.3333	0.0502	0.0251	0.0125	0.0251	0.0502
12	0.0361	0.0722	0.1443	0.0722	0.0361	0.0180	0.2887	0.1667	0.0962	0.1925	0.3333	0.0000	0.0869	0.0434	0.0217	0.0434	0.0869
13	0.0752	0.1505	0.3010	0.6019	0.3010	0.1505	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.0000	0.3623	0.1812	0.0906	0.1812
14	0.1505	0.0752	0.1505	0.3010	0.6019	0.3010	0.0752	0.0434	0.0251	0.0145	0.0251	0.0434	0.3623	0.0000	0.3623	0.1812	0.0906
15	0.3010	0.1505	0.0752	0.1505	0.3010	0.6019	0.0376	0.0217	0.0125	0.0072	0.0125	0.0217	0.1812	0.3623	0.0000	0.3623	0.1812
16	0.6019	0.3010	0.1505	0.0752	0.1505	0.3010	0.0752	0.0434	0.0251	0.0145	0.0251	0.0434	0.0906	0.1812	0.3623	0.0000	0.3623
17	0.3010	0.6019	0.3010	0.1505	0.0752	0.1505	0.1505	0.0869	0.0502	0.0290	0.0502	0.0869	0.1812	0.0906	0.1812	0.3623	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2500	0.1250	0.0722	0.1443	0.2500	0.0625	0.0313	0.0180	0.0090	0.0208	0.0361	0.3010	0.6019	0.3010	0.0376	0.0109
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1250	0.1250	0.0625	0.0361	0.0180	0.0417	0.0722	0.1505	0.3010	0.6019	0.0752	0.0217
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1250	0.0722	0.0361	0.0833	0.1443	0.1003	0.1505	0.3010	0.1505	0.0434
4	0.0833	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0722	0.0417	0.0208	0.0481	0.0833	0.2006	0.1003	0.1738	0.0869	0.0251
5	0.1443	0.0722	0.1667	0.3333	0.0000	0.2887	0.0833	0.0417	0.0241	0.0120	0.0278	0.0481	0.3475	0.1738	0.0869	0.0502	0.0145
6	0.2500	0.1250	0.0625	0.1667	0.2887	0.0000	0.0313	0.0156	0.0090	0.0045	0.0104	0.0180	0.6019	0.3010	0.1505	0.0188	0.0054
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2500	0.1443	0.0722	0.1667	0.2887	0.0502	0.0752	0.1505	0.3010	0.0869
8	0.0313	0.0625	0.1250	0.0722	0.0417	0.0208	0.2500	0.0000	0.2887	0.1443	0.0833	0.1443	0.0251	0.0376	0.0752	0.6019	0.1738
9	0.0180	0.0361	0.0722	0.0417	0.0241	0.0120	0.1443	0.2887	0.0000	0.2887	0.1667	0.0962	0.0145	0.0217	0.0434	0.3475	0.3475
10	0.0104	0.0208	0.0417	0.0241	0.0139	0.0069	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.0084	0.0125	0.0251	0.1738	0.6019
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0833	0.1667	0.2887	0.0000	0.3333	0.0167	0.0251	0.0502	0.1003	0.3475
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1443	0.0962	0.1667	0.3333	0.0000	0.0290	0.0434	0.0869	0.1738	0.2006
13	0.3010	0.1505	0.0752	0.2006	0.3475	0.6019	0.0376	0.0188	0.0109	0.0054	0.0125	0.0217	0.0000	0.3623	0.1812	0.0226	0.0065
14	0.6019	0.3010	0.1505	0.0869	0.1738	0.3010	0.0752	0.0376	0.0217	0.0109	0.0251	0.0434	0.3623	0.0000	0.3623	0.0453	0.0131
15	0.3010	0.6019	0.3010	0.1738	0.1003	0.1505	0.1505	0.0752	0.0434	0.0217	0.0502	0.0869	0.1812	0.3623	0.0000	0.0906	0.0261
16	0.0376	0.0752	0.1505	0.0869	0.0502	0.0251	0.3010	0.6019	0.3475	0.1738	0.1003	0.1738	0.0302	0.0453	0.0906	0.0000	0.2092
17	0.0125	0.0251	0.0502	0.0290	0.0167	0.0084	0.1003	0.1738	0.3475	0.6019	0.4184	0.2006	0.0101	0.0151	0.0302	0.2092	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2500	0.1250	0.0625	0.1667	0.2887	0.0625	0.0313	0.0180	0.0104	0.0180	0.0361	0.6019	0.3010	0.0376	0.0752	0.0217
2	0.2500	0.0000	0.2500	0.1250	0.0722	0.1443	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.3010	0.6019	0.0752	0.1505	0.0434
3	0.1250	0.2500	0.0000	0.2500	0.1443	0.0833	0.2500	0.1250	0.0722	0.0417	0.0722	0.1443	0.1505	0.3010	0.1505	0.3010	0.0869
4	0.0833	0.1250	0.2500	0.0000	0.2887	0.1667	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.1003	0.1505	0.0752	0.6019	0.0434
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.3333	0.0722	0.0361	0.0208	0.0120	0.0208	0.0417	0.2006	0.1003	0.0434	0.3475	0.0251
6	0.2887	0.1443	0.0722	0.1667	0.3333	0.0000	0.0361	0.0180	0.0104	0.0060	0.0104	0.0208	0.3475	0.1738	0.0217	0.2006	0.0125
7	0.0625	0.1250	0.2500	0.1250	0.0722	0.0417	0.0000	0.2500	0.1443	0.0833	0.1443	0.2887	0.0752	0.1505	0.3010	0.1505	0.1738
8	0.0313	0.0625	0.1250	0.0625	0.0361	0.0208	0.2500	0.0000	0.2887	0.1667	0.0833	0.1443	0.0376	0.0752	0.6019	0.0752	0.1003
9	0.0180	0.0361	0.0722	0.0361	0.0208	0.0120	0.1443	0.2887	0.0000	0.3333	0.1667	0.0962	0.0217	0.0434	0.3475	0.0434	0.2006
10	0.0069	0.0208	0.0417	0.0208	0.0120	0.0069	0.0833	0.1667	0.3333	0.0000	0.2887	0.1667	0.0084	0.0251	0.2006	0.0251	0.3475
11	0.0180	0.0361	0.0722	0.0361	0.0241	0.0120	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0217	0.0434	0.0869	0.0434	0.6019
12	0.0361	0.0722	0.1443	0.0722	0.0417	0.0241	0.2887	0.1443	0.0833	0.1667	0.2887	0.0000	0.0434	0.0869	0.1738	0.0869	0.3475
13	0.6019	0.3010	0.1505	0.0752	0.2006	0.3475	0.0752	0.0376	0.0217	0.0125	0.0217	0.0434	0.0000	0.3623	0.0453	0.0906	0.0261
14	0.3010	0.6019	0.3010	0.1505	0.0869	0.1738	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.3623	0.0000	0.0906	0.1812	0.0523
15	0.0376	0.0752	0.1505	0.0752	0.0434	0.0251	0.3010	0.6019	0.3475	0.2006	0.1003	0.1738	0.0453	0.0906	0.0000	0.0906	0.1208
16	0.1003	0.1505	0.3010	0.6019	0.3475	0.2006	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.1208	0.1812	0.0906	0.0000	0.0523
17	0.0217	0.0434	0.0869	0.0434	0.0290	0.0145	0.1738	0.0869	0.2006	0.3475	0.6019	0.3475	0.0261	0.0523	0.1046	0.0523	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.0722	0.0361	0.0208	0.0120	0.0241	0.0361	0.3475	0.0434	0.0869	0.3475	0.0434
2	0.2887	0.0000	0.2500	0.1250	0.0722	0.1443	0.1250	0.0625	0.0361	0.0208	0.0361	0.0625	0.6019	0.0752	0.1505	0.1738	0.0752
3	0.1443	0.2500	0.0000	0.2500	0.1443	0.0722	0.2500	0.1250	0.0722	0.0417	0.0722	0.1250	0.3010	0.1505	0.3010	0.0869	0.1505
4	0.0833	0.1250	0.2500	0.0000	0.2887	0.1443	0.1250	0.0625	0.0361	0.0208	0.0361	0.0625	0.1505	0.0752	0.6019	0.1738	0.0752
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0208	0.0120	0.0123	0.0361	0.1003	0.0434	0.3475	0.3475	0.0434
6	0.2887	0.1443	0.0722	0.1443	0.2887	0.0000	0.0361	0.0180	0.0104	0.0060	0.0104	0.0180	0.1738	0.0217	0.1738	0.6019	0.0217
7	0.0722	0.1250	0.2500	0.1250	0.0722	0.0361	0.0000	0.2500	0.1443	0.0833	0.1443	0.2500	0.1505	0.3010	0.1505	0.0434	0.3010
8	0.0361	0.0625	0.1250	0.0625	0.0163	0.0180	0.2500	0.0000	0.2887	0.1667	0.0962	0.1250	0.0752	0.6019	0.0752	0.0217	0.1505
9	0.0208	0.0361	0.0722	0.0361	0.0208	0.0104	0.1443	0.2887	0.0000	0.3333	0.1925	0.0962	0.0434	0.3475	0.0434	0.0125	0.1158
10	0.0120	0.0208	0.0417	0.0208	0.0120	0.0060	0.0833	0.1667	0.3333	0.0000	0.3333	0.1667	0.0251	0.2006	0.0251	0.0072	0.2006
11	0.0208	0.0361	0.0722	0.0361	0.0208	0.0104	0.1443	0.0722	0.1925	0.3333	0.0000	0.2887	0.0434	0.0869	0.0434	0.0125	0.3475
12	0.0361	0.0625	0.1250	0.0625	0.0361	0.0180	0.2500	0.1250	0.0722	0.1667	0.2887	0.0000	0.0752	0.1505	0.0752	0.0217	0.6019
13	0.3475	0.6019	0.3010	0.1505	0.0869	0.1738	0.1505	0.0752	0.0434	0.0251	0.0434	0.0752	0.0000	0.0906	0.1812	0.2092	0.0906
14	0.0434	0.0752	0.1505	0.0752	0.0196	0.0217	0.3010	0.6019	0.3475	0.2006	0.1158	0.1505	0.0906	0.0000	0.0906	0.0261	0.1812
15	0.1003	0.1505	0.3010	0.6019	0.3475	0.1738	0.1505	0.0752	0.0434	0.0251	0.0434	0.0752	0.1812	0.0906	0.0000	0.2092	0.0906
16	0.3475	0.1738	0.0869	0.1738	0.3475	0.6019	0.0434	0.0217	0.0125	0.0072	0.0125	0.0217	0.2092	0.0261	0.2092	0.0000	0.0261
17	0.0434	0.0752	0.1505	0.0752	0.0434	0.0217	0.3010	0.1505	0.0869	0.2006	0.3475	0.6019	0.0906	0.1812	0.0906	0.0261	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2500	0.1250	0.0722	0.1443	0.2500	0.0625	0.0313	0.0180	0.0104	0.0180	0.0361	0.3010	0.6019	0.3010	0.0376	0.0217
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1250	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.1505	0.3010	0.6019	0.0752	0.0434
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1250	0.0722	0.0417	0.0722	0.1443	0.1003	0.1505	0.3010	0.1505	0.0869
4	0.0833	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0722	0.0417	0.0241	0.0417	0.0833	0.2006	0.1003	0.1738	0.0869	0.0502
5	0.1443	0.0722	0.1667	0.3333	0.0000	0.2887	0.0833	0.0417	0.0241	0.0139	0.0241	0.0481	0.3475	0.1738	0.0869	0.0502	0.0290
6	0.2500	0.1250	0.0625	0.1667	0.2887	0.0000	0.0313	0.0156	0.0090	0.0052	0.0090	0.0180	0.6019	0.3010	0.1505	0.0188	0.0109
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2500	0.1443	0.0833	0.1443	0.2887	0.0502	0.0752	0.1505	0.3010	0.1738
8	0.0313	0.0625	0.1250	0.0722	0.0417	0.0208	0.2500	0.0000	0.2887	0.1667	0.0833	0.1443	0.0251	0.0376	0.0752	0.6019	0.1003
9	0.0180	0.0361	0.0722	0.0417	0.0241	0.0120	0.1443	0.2887	0.0000	0.3333	0.1667	0.0962	0.0145	0.0217	0.0434	0.3475	0.2006
10	0.0104	0.0208	0.0417	0.0241	0.0139	0.0069	0.0833	0.1667	0.3333	0.0000	0.2887	0.1667	0.0084	0.0125	0.0251	0.2006	0.3475
11	0.0180	0.0361	0.0722	0.0417	0.0241	0.0120	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0145	0.0217	0.0434	0.0869	0.6019
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1443	0.0833	0.1667	0.2887	0.0000	0.0290	0.0434	0.0869	0.1738	0.3475
13	0.3010	0.1505	0.0752	0.2006	0.3475	0.6019	0.0376	0.0188	0.0109	0.0063	0.0109	0.0217	0.0000	0.3623	0.1812	0.0226	0.0131
14	0.6019	0.3010	0.1505	0.0869	0.1738	0.3010	0.0752	0.0376	0.0217	0.0125	0.0217	0.0434	0.3623	0.0000	0.3623	0.0453	0.0261
15	0.3010	0.6019	0.3010	0.1738	0.1003	0.1505	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.1812	0.3623	0.0000	0.0906	0.0523
16	0.0376	0.0752	0.1505	0.0869	0.0502	0.0251	0.3010	0.6019	0.3475	0.2006	0.1003	0.1738	0.0302	0.0453	0.0906	0.0000	0.1208
17	0.0217	0.0434	0.0869	0.0502	0.0290	0.0145	0.1738	0.0869	0.2006	0.3475	0.6019	0.3475	0.0174	0.0261	0.0523	0.1046	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0361	0.0180	0.0104	0.0241	0.0417	0.3475	0.0434	0.0217	0.3475	0.1738
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0625	0.0313	0.0180	0.0417	0.0722	0.6019	0.0752	0.0376	0.1738	0.0869
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0625	0.0361	0.0833	0.1443	0.3010	0.1505	0.0752	0.0869	0.1738
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0361	0.0208	0.0481	0.0833	0.1738	0.0869	0.0434	0.1738	0.3475
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0180	0.0104	0.0241	0.0417	0.0869	0.0434	0.0217	0.3010	0.6019
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0180	0.0090	0.0052	0.0120	0.0208	0.1738	0.0217	0.0109	0.6019	0.3010
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1250	0.0722	0.1667	0.2887	0.1505	0.3010	0.1505	0.0434	0.0869
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2500	0.1443	0.0833	0.1443	0.0752	0.6019	0.3010	0.0217	0.0434
9	0.0180	0.0313	0.0625	0.0361	0.0180	0.0090	0.1250	0.2500	0.0000	0.2887	0.1667	0.0962	0.0376	0.3010	0.6019	0.0109	0.0217
10	0.0139	0.0241	0.0481	0.0278	0.0139	0.0069	0.0962	0.1443	0.2887	0.0000	0.3333	0.1925	0.0290	0.1738	0.3475	0.0084	0.0167
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0833	0.1667	0.3333	0.0000	0.3333	0.0502	0.1003	0.2006	0.0145	0.0290
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0722	0.1925	0.3333	0.0000	0.0869	0.1738	0.0869	0.0251	0.0502
13	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0752	0.0376	0.0217	0.0502	0.0869	0.0000	0.0906	0.0453	0.2092	0.1046
14	0.0434	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3010	0.1738	0.1003	0.1738	0.0906	0.0000	0.3623	0.0261	0.0523
15	0.0217	0.0376	0.0752	0.0434	0.0217	0.0109	0.1505	0.3010	0.6019	0.3475	0.2006	0.1158	0.0453	0.3623	0.0000	0.0131	0.0261
16	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0217	0.0109	0.0063	0.0145	0.0251	0.2092	0.0261	0.0131	0.0000	0.3623
17	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0217	0.0125	0.0290	0.0502	0.1046	0.0523	0.0261	0.3623	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0361	0.0208	0.0104	0.0241	0.0417	0.1738	0.3475	0.3475	0.0434	0.0125
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0625	0.0361	0.0180	0.0417	0.0722	0.0869	0.1738	0.6019	0.0752	0.0217
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0722	0.0361	0.0833	0.1443	0.1738	0.0869	0.3010	0.1505	0.0434
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0417	0.0208	0.0481	0.0833	0.3475	0.1738	0.1738	0.0869	0.0251
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0208	0.0104	0.0241	0.0417	0.6019	0.3010	0.0869	0.0434	0.0125
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0180	0.0104	0.0052	0.0120	0.0208	0.3010	0.6019	0.1738	0.0217	0.0063
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1443	0.0722	0.1667	0.2887	0.0869	0.0434	0.1505	0.3010	0.0869
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2887	0.1443	0.0833	0.1443	0.0434	0.0217	0.0752	0.6019	0.1738
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.2887	0.1667	0.0962	0.0251	0.0125	0.0434	0.3475	0.3475
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0060	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.0145	0.0072	0.0251	0.1738	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0833	0.1667	0.2887	0.0000	0.3333	0.0290	0.0145	0.0502	0.1003	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0833	0.1667	0.3333	0.0000	0.0502	0.0251	0.0869	0.1738	0.2006
13	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0251	0.0125	0.0290	0.0502	0.0000	0.3623	0.1046	0.0523	0.0151
14	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0217	0.0125	0.0063	0.0145	0.0251	0.3623	0.0000	0.2092	0.0261	0.0075
15	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0752	0.0434	0.0217	0.0502	0.0869	0.1046	0.2092	0.0000	0.0906	0.0261
16	0.0434	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3475	0.1738	0.1003	0.1738	0.0523	0.0261	0.0906	0.0000	0.2092
17	0.0145	0.0251	0.0502	0.0290	0.0145	0.0072	0.1003	0.1738	0.3475	0.6019	0.3475	0.2006	0.0174	0.0087	0.0302	0.2092	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0361	0.0208	0.0120	0.0208	0.0417	0.1738	0.3475	0.3475	0.0434	0.0251
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.0869	0.1738	0.6019	0.0752	0.0434
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0722	0.0417	0.0722	0.1443	0.1738	0.0869	0.3010	0.1505	0.0869
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0417	0.0241	0.0417	0.0833	0.3475	0.1738	0.1738	0.0869	0.0502
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0208	0.0120	0.0208	0.0417	0.6019	0.3010	0.0869	0.0434	0.0251
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0180	0.0104	0.0060	0.0104	0.0208	0.3010	0.6019	0.1738	0.0217	0.0125
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1443	0.0833	0.1443	0.2887	0.0869	0.0434	0.1505	0.3010	0.1738
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2887	0.1667	0.0833	0.1443	0.0434	0.0217	0.0752	0.6019	0.1003
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.3333	0.1667	0.0962	0.0251	0.0125	0.0434	0.3475	0.2006
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0060	0.0833	0.1667	0.3333	0.0000	0.2887	0.1667	0.0145	0.0072	0.0251	0.2006	0.3475
11	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0251	0.0125	0.0434	0.0869	0.6019
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0833	0.1667	0.2887	0.0000	0.0502	0.0251	0.0869	0.1738	0.3475
13	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0251	0.0145	0.0251	0.0502	0.0000	0.3623	0.1046	0.0523	0.0302
14	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0217	0.0125	0.0072	0.0125	0.0251	0.3623	0.0000	0.2092	0.0261	0.0151
15	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.1046	0.2092	0.0000	0.0906	0.0523
16	0.0434	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3475	0.2006	0.1003	0.1738	0.0523	0.0261	0.0906	0.0000	0.1208
17	0.0251	0.0434	0.0869	0.0502	0.0251	0.0125	0.1738	0.0869	0.2006	0.3475	0.6019	0.3475	0.0302	0.0151	0.0523	0.1046	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2500	0.1250	0.0625	0.1667	0.2887	0.0625	0.0361	0.0180	0.0090	0.0208	0.0361	0.0752	0.6019	0.3010	0.0217	0.0109
2	0.2500	0.0000	0.2500	0.1250	0.0722	0.1443	0.1250	0.0722	0.0361	0.0180	0.0417	0.0722	0.1505	0.3010	0.6019	0.0434	0.0217
3	0.1250	0.2500	0.0000	0.2500	0.1443	0.0833	0.2500	0.1443	0.0722	0.0361	0.0833	0.1443	0.3010	0.1505	0.3010	0.0869	0.0434
4	0.0833	0.1250	0.2500	0.0000	0.2887	0.1667	0.1250	0.0722	0.0361	0.0180	0.0417	0.0722	0.6019	0.1003	0.1505	0.0434	0.0217
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.3333	0.0722	0.0417	0.0208	0.0104	0.0241	0.0417	0.3475	0.2006	0.1003	0.0251	0.0125
6	0.2887	0.1443	0.0722	0.1667	0.3333	0.0000	0.0361	0.0208	0.0104	0.0052	0.0120	0.0208	0.2006	0.3475	0.1738	0.0125	0.0063
7	0.0625	0.1250	0.2500	0.1250	0.0722	0.0417	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.1505	0.0752	0.1505	0.1738	0.0869
8	0.0361	0.0722	0.1443	0.0722	0.0417	0.0241	0.2887	0.0000	0.2887	0.1443	0.0833	0.1667	0.0869	0.0434	0.0869	0.3475	0.1738
9	0.0180	0.0361	0.0722	0.0361	0.0208	0.0120	0.1443	0.2887	0.0000	0.2500	0.1443	0.0833	0.0434	0.0217	0.0434	0.6019	0.3010
10	0.0104	0.0208	0.0417	0.0208	0.0120	0.0069	0.0833	0.1443	0.2500	0.0000	0.2887	0.1667	0.0251	0.0125	0.0251	0.3010	0.6019
11	0.0208	0.0417	0.0833	0.0417	0.0241	0.0139	0.1667	0.0962	0.1443	0.2887	0.0000	0.3333	0.0502	0.0251	0.0502	0.1738	0.3475
12	0.0361	0.0722	0.1443	0.0722	0.0417	0.0241	0.2887	0.1667	0.0833	0.1667	0.3333	0.0000	0.0869	0.0434	0.0869	0.1003	0.2006
13	0.1003	0.1505	0.3010	0.6019	0.3475	0.2006	0.1505	0.0869	0.0434	0.0217	0.0502	0.0869	0.0000	0.1208	0.1812	0.0523	0.0261
14	0.6019	0.3010	0.1505	0.0752	0.2006	0.3475	0.0752	0.0434	0.0217	0.0109	0.0251	0.0434	0.0906	0.0000	0.3623	0.0261	0.0131
15	0.3010	0.6019	0.3010	0.1505	0.0869	0.1738	0.1505	0.0869	0.0434	0.0217	0.0502	0.0869	0.1812	0.3623	0.0000	0.0523	0.0261
16	0.0217	0.0434	0.0869	0.0434	0.0251	0.0145	0.1738	0.3475	0.6019	0.3010	0.1738	0.1003	0.0523	0.0261	0.0523	0.0000	0.3623
17	0.0125	0.0251	0.0502	0.0251	0.0145	0.0084	0.1003	0.1738	0.3010	0.6019	0.3475	0.2006	0.0302	0.0151	0.0302	0.3623	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0417	0.0208	0.0104	0.0241	0.0417	0.1738	0.3475	0.3475	0.0251	0.0125
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0722	0.0361	0.0180	0.0417	0.0722	0.0869	0.1738	0.6019	0.0434	0.0217
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1443	0.0722	0.0361	0.0833	0.1443	0.1738	0.0869	0.3010	0.0869	0.0434
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0833	0.0417	0.0208	0.0481	0.0833	0.3475	0.1738	0.1738	0.0502	0.0251
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0417	0.0208	0.0104	0.0241	0.0417	0.6019	0.3010	0.0869	0.0251	0.0125
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0208	0.0104	0.0052	0.0120	0.0208	0.3010	0.6019	0.1738	0.0125	0.0063
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.0869	0.0434	0.1505	0.1738	0.0869
8	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.0000	0.2887	0.1443	0.0833	0.1667	0.0502	0.0251	0.0869	0.3475	0.1738
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.2500	0.1443	0.0833	0.0251	0.0125	0.0434	0.6019	0.3010
10	0.0120	0.0208	0.0417	0.0241	0.0120	0.0060	0.0833	0.1443	0.2500	0.0000	0.2887	0.1667	0.0145	0.0072	0.0251	0.3010	0.6019
11	0.0241	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0962	0.1443	0.2887	0.0000	0.3333	0.0290	0.0145	0.0502	0.1738	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1667	0.0833	0.1667	0.3333	0.0000	0.0502	0.0251	0.0869	0.1003	0.2006
13	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0502	0.0251	0.0125	0.0290	0.0502	0.0000	0.3623	0.1046	0.0302	0.0151
14	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0251	0.0125	0.0063	0.0145	0.0251	0.3623	0.0000	0.2092	0.0151	0.0075
15	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0869	0.0434	0.0217	0.0502	0.0869	0.1046	0.2092	0.0000	0.0523	0.0261
16	0.0251	0.0434	0.0869	0.0502	0.0251	0.0125	0.1738	0.3475	0.6019	0.3010	0.1738	0.1003	0.0302	0.0151	0.0523	0.0000	0.3623
17	0.0145	0.0251	0.0502	0.0290	0.0145	0.0072	0.1003	0.1738	0.3010	0.6019	0.3475	0.2006	0.0174	0.0087	0.0302	0.3623	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2500	0.1250	0.0625	0.1667	0.2887	0.0625	0.0313	0.0156	0.0090	0.0180	0.0313	0.0752	0.6019	0.3010	0.0376	0.0188	0.0376
2	0.2500	0.0000	0.2500	0.1250	0.0722	0.1443	0.1250	0.0625	0.0313	0.0180	0.0361	0.0625	0.1505	0.3010	0.6019	0.0752	0.0376	0.0752
3	0.1250	0.2500	0.0000	0.2500	0.1443	0.0833	0.2500	0.1250	0.0625	0.0163	0.0722	0.1250	0.3010	0.1505	0.3010	0.1505	0.0752	0.1505
4	0.0833	0.1250	0.2500	0.0000	0.2887	0.1667	0.1250	0.0625	0.0313	0.0180	0.0361	0.0625	0.6019	0.1003	0.1505	0.0752	0.0376	0.0752
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.3333	0.0722	0.0361	0.0180	0.0104	0.0208	0.0361	0.3475	0.2006	0.1003	0.0434	0.0217	0.0434
6	0.2887	0.1443	0.0722	0.1667	0.3333	0.0000	0.0361	0.0180	0.0090	0.0052	0.0104	0.0180	0.2006	0.3475	0.1738	0.0217	0.0109	0.0217
7	0.0625	0.1250	0.2500	0.1250	0.0722	0.0417	0.0000	0.2500	0.1250	0.0722	0.1443	0.2500	0.1505	0.0752	0.1505	0.3010	0.1505	0.3010
8	0.0313	0.0625	0.1250	0.0625	0.0361	0.0208	0.2500	0.0000	0.2500	0.1443	0.0833	0.1250	0.0752	0.0376	0.0752	0.6019	0.3010	0.1505
9	0.0156	0.0313	0.0625	0.0313	0.0180	0.0104	0.1250	0.2500	0.0000	0.2887	0.1667	0.0833	0.0376	0.0188	0.0376	0.3010	0.6019	0.1003
10	0.0104	0.0208	0.0417	0.0208	0.0120	0.0069	0.0833	0.1443	0.2887	0.0000	0.3333	0.1667	0.0251	0.0125	0.0251	0.1738	0.3475	0.2006
11	0.0180	0.0361	0.0722	0.0361	0.0208	0.0120	0.1443	0.0722	0.1667	0.3333	0.0000	0.2887	0.0434	0.0217	0.0434	0.0869	0.2006	0.3475
12	0.0313	0.0625	0.1250	0.0625	0.0361	0.0208	0.2500	0.1250	0.0625	0.1667	0.2887	0.0000	0.0752	0.0376	0.0752	0.1505	0.0752	0.6019
13	0.1003	0.1505	0.3010	0.6019	0.3475	0.2006	0.1505	0.0752	0.0376	0.0217	0.0434	0.0752	0.0000	0.1208	0.1812	0.0906	0.0453	0.0906
14	0.6019	0.3010	0.1505	0.0752	0.2006	0.3475	0.0752	0.0376	0.0188	0.0109	0.0217	0.0376	0.0906	0.0000	0.3623	0.0453	0.0226	0.0453
15	0.3010	0.6019	0.3010	0.1505	0.0869	0.1738	0.1505	0.0752	0.0376	0.0217	0.0434	0.0752	0.1812	0.3623	0.0000	0.0906	0.0453	0.0906
16	0.0376	0.0752	0.1505	0.0752	0.0434	0.0251	0.3010	0.6019	0.3010	0.1738	0.1003	0.1505	0.0906	0.0453	0.0906	0.0000	0.3623	0.1812
17	0.0188	0.0376	0.0752	0.0376	0.0217	0.0125	0.1505	0.3010	0.6019	0.3475	0.2006	0.1003	0.0453	0.0226	0.0453	0.3623	0.0000	0.1208
18	0.0376	0.0752	0.1505	0.0752	0.0434	0.0251	0.3010	0.1505	0.0752	0.2006	0.3475	0.6019	0.0906	0.0453	0.0906	0.1812	0.0906	0.0000

2-2'-3-4'-5-5'-HEXACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2500	0.1250	0.0722	0.1443	0.2887	0.0625	0.0313	0.0180	0.0090	0.0180	0.0361	0.1738	0.6019	0.3010	0.0376	0.0109	0.0217
2	0.2500	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0625	0.0361	0.0180	0.0361	0.0722	0.0869	0.3010	0.6019	0.0752	0.0217	0.0434
3	0.1250	0.2500	0.0000	0.2887	0.1443	0.0833	0.2500	0.1250	0.0722	0.0361	0.0722	0.1443	0.1738	0.1505	0.3010	0.1505	0.0434	0.0869
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.1443	0.0722	0.0417	0.0208	0.0417	0.0833	0.3475	0.1003	0.1738	0.0869	0.0251	0.0502
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0208	0.0104	0.0208	0.0417	0.6019	0.1738	0.0869	0.0434	0.0125	0.0251
6	0.2887	0.1443	0.0722	0.1667	0.2887	0.0000	0.0361	0.0180	0.0104	0.0052	0.0104	0.0208	0.3475	0.3475	0.1738	0.0217	0.0063	0.0125
7	0.0625	0.1250	0.2500	0.1443	0.0722	0.0417	0.0000	0.2500	0.1443	0.0722	0.1443	0.2887	0.0869	0.0752	0.1505	0.3010	0.0869	0.1738
8	0.0313	0.0625	0.1250	0.0722	0.0361	0.0208	0.2500	0.0000	0.2887	0.1443	0.0722	0.1443	0.0434	0.0376	0.0752	0.6019	0.1738	0.0869
9	0.0180	0.0361	0.0722	0.0417	0.0208	0.0120	0.1443	0.2887	0.0000	0.2887	0.1443	0.0833	0.0251	0.0217	0.0434	0.3475	0.3475	0.1738
10	0.0090	0.0180	0.0361	0.0208	0.0104	0.0060	0.0722	0.1443	0.2887	0.0000	0.2500	0.1443	0.0125	0.0109	0.0217	0.1738	0.6019	0.3010
11	0.0180	0.0361	0.0722	0.0417	0.0208	0.0120	0.1443	0.0722	0.1443	0.2500	0.0000	0.2887	0.0251	0.0217	0.0434	0.0869	0.3010	0.6019
12	0.0361	0.0722	0.1443	0.0833	0.0417	0.0241	0.2887	0.1443	0.0833	0.1443	0.2887	0.0000	0.0502	0.0434	0.0869	0.1738	0.1738	0.3475
13	0.1738	0.0869	0.1738	0.3475	0.6019	0.3475	0.0869	0.0434	0.0251	0.0125	0.0251	0.0502	0.0000	0.2092	0.1046	0.0523	0.0151	0.0302
14	0.6019	0.3010	0.1505	0.0869	0.1738	0.3475	0.0752	0.0434	0.0251	0.0125	0.0251	0.0502	0.2092	0.0000	0.3623	0.0453	0.0131	0.0261
15	0.3010	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0752	0.0434	0.0217	0.0434	0.0869	0.1046	0.3623	0.0000	0.0906	0.0261	0.0523
16	0.0376	0.0752	0.1505	0.0869	0.0434	0.0251	0.3010	0.6019	0.3475	0.1738	0.0869	0.1738	0.0523	0.0453	0.0906	0.0000	0.2092	0.1046
17	0.0109	0.0217	0.0434	0.0251	0.0125	0.0072	0.0869	0.1738	0.3475	0.6019	0.3010	0.1738	0.0151	0.0131	0.0261	0.2092	0.0000	0.3623
18	0.0217	0.0434	0.0869	0.0502	0.0251	0.0145	0.1738	0.0869	0.1738	0.3010	0.6019	0.3475	0.0302	0.0261	0.0523	0.1046	0.3623	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2500	0.1250	0.0722	0.1250	0.2500	0.0625	0.0313	0.0180	0.0090	0.0208	0.0361	0.1505	0.3010	0.6019	0.3010	0.0376	0.0109
2	0.2500	0.0000	0.2500	0.1443	0.0722	0.1250	0.1250	0.0625	0.0361	0.0180	0.0417	0.0722	0.0869	0.1505	0.3010	0.6019	0.0752	0.0217
3	0.1250	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0722	0.0361	0.0833	0.1443	0.1738	0.0869	0.1505	0.3010	0.1505	0.0434
4	0.0722	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0417	0.0208	0.0481	0.0833	0.3475	0.1738	0.0869	0.1738	0.0869	0.0251
5	0.1250	0.0625	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0208	0.0104	0.0241	0.0417	0.6019	0.3010	0.1505	0.0752	0.0434	0.0125
6	0.2500	0.1250	0.0625	0.1443	0.2500	0.0000	0.0313	0.0156	0.0090	0.0045	0.0104	0.0180	0.3010	0.6019	0.3010	0.1505	0.0188	0.0054
7	0.0625	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1443	0.0722	0.1667	0.2887	0.0869	0.0434	0.0752	0.1505	0.3010	0.0869
8	0.0313	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2887	0.1443	0.0833	0.1443	0.0434	0.0217	0.0376	0.0752	0.6019	0.1738
9	0.0180	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.2887	0.1667	0.0962	0.0251	0.0125	0.0217	0.0434	0.3475	0.3475
10	0.0104	0.0208	0.0417	0.0241	0.0120	0.0060	0.0833	0.1443	0.2887	0.0000	0.2887	0.1667	0.0145	0.0072	0.0125	0.0251	0.1738	0.6019
11	0.0208	0.0417	0.0833	0.0481	0.0241	0.0120	0.1667	0.0833	0.1667	0.2887	0.0000	0.3333	0.0290	0.0145	0.0251	0.0502	0.1003	0.3475
12	0.0361	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0833	0.1667	0.3333	0.0000	0.0502	0.0251	0.0434	0.0869	0.1738	0.2006
13	0.1505	0.0752	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0251	0.0125	0.0290	0.0502	0.0000	0.3623	0.1812	0.0906	0.0523	0.0151
14	0.3010	0.1505	0.0752	0.1738	0.3010	0.6019	0.0376	0.0188	0.0109	0.0054	0.0125	0.0217	0.3623	0.0000	0.3623	0.1812	0.0226	0.0065
15	0.6019	0.3010	0.1505	0.0869	0.1505	0.3010	0.0752	0.0376	0.0217	0.0109	0.0251	0.0434	0.1812	0.3623	0.0000	0.3623	0.0453	0.0109
16	0.3010	0.6019	0.3010	0.1738	0.0869	0.1505	0.1505	0.0752	0.0434	0.0217	0.0502	0.0869	0.1046	0.1812	0.3623	0.0000	0.0906	0.0261
17	0.0376	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3475	0.1738	0.1003	0.1738	0.0523	0.0261	0.0453	0.0906	0.0000	0.2092
18	0.0125	0.0251	0.0502	0.0290	0.0145	0.0072	0.1003	0.1738	0.3475	0.6019	0.3475	0.2006	0.0174	0.0087	0.0151	0.0302	0.2092	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2500	0.1250	0.0722	0.1250	0.2500	0.0625	0.0313	0.0180	0.0104	0.0180	0.0361	0.1505	0.3010	0.6019	0.3010	0.0376	0.0217
2	0.2500	0.0000	0.2500	0.1443	0.0722	0.1250	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.0869	0.1505	0.3010	0.6019	0.0752	0.0434
3	0.1250	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0722	0.0417	0.0722	0.1443	0.1738	0.0869	0.1505	0.3010	0.1505	0.0869
4	0.0722	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0417	0.0241	0.0417	0.0833	0.3475	0.1738	0.0869	0.1738	0.0869	0.0502
5	0.1250	0.0625	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0208	0.0120	0.0208	0.0417	0.6019	0.3010	0.1505	0.0752	0.0434	0.0251
6	0.2500	0.1250	0.0625	0.1443	0.2500	0.0000	0.0313	0.0156	0.0090	0.0052	0.0090	0.0180	0.3010	0.6019	0.3010	0.1505	0.0188	0.0109
7	0.0625	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1443	0.0833	0.1443	0.2887	0.0869	0.0434	0.0752	0.1505	0.3010	0.1738
8	0.0313	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2887	0.1667	0.0833	0.1443	0.0434	0.0217	0.0376	0.0752	0.6019	0.1003
9	0.0180	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.3333	0.1667	0.0962	0.0251	0.0125	0.0217	0.0434	0.3475	0.2006
10	0.0104	0.0208	0.0481	0.0241	0.0120	0.0060	0.0833	0.1667	0.3333	0.0000	0.2887	0.1667	0.0145	0.0072	0.0125	0.0251	0.2006	0.3475
11	0.0180	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0251	0.0125	0.0217	0.0434	0.0869	0.6019
12	0.0361	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0833	0.1667	0.2887	0.0000	0.0502	0.0251	0.0434	0.0869	0.1738	0.3475
13	0.1505	0.0752	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0251	0.0145	0.0251	0.0502	0.0000	0.3623	0.1812	0.0906	0.0523	0.0302
14	0.3010	0.1505	0.0752	0.1738	0.3010	0.6019	0.0376	0.0188	0.0109	0.0063	0.0109	0.0217	0.3623	0.0000	0.3623	0.1812	0.0226	0.0131
15	0.6019	0.3010	0.1505	0.0869	0.1505	0.3010	0.0752	0.0376	0.0217	0.0125	0.0217	0.0434	0.1812	0.3623	0.0000	0.3623	0.0453	0.0261
16	0.3010	0.6019	0.3010	0.1738	0.0869	0.1505	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.1046	0.1812	0.3623	0.0000	0.0906	0.0523
17	0.0376	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3475	0.2006	0.1003	0.1738	0.0523	0.0261	0.0453	0.0906	0.0000	0.1208
18	0.0217	0.0434	0.0869	0.0502	0.0251	0.0125	0.1738	0.0869	0.2006	0.3475	0.6019	0.3475	0.0302	0.0151	0.0261	0.0523	0.1046	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0361	0.0208	0.0104	0.0208	0.0417	0.1738	0.3475	0.3475	0.0434	0.0125	0.0251
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0625	0.0361	0.0180	0.0361	0.0722	0.0869	0.1738	0.6019	0.0752	0.0217	0.0434
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0722	0.0361	0.0722	0.1443	0.1738	0.0869	0.3010	0.1505	0.0434	0.0869
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0417	0.0208	0.0417	0.0833	0.3475	0.1738	0.1738	0.0869	0.0251	0.0502
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0208	0.0104	0.0208	0.0417	0.6019	0.3010	0.0869	0.0434	0.0125	0.0251
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0180	0.0104	0.0052	0.0104	0.0208	0.3010	0.6019	0.1738	0.0217	0.0063	0.0125
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1443	0.0722	0.1443	0.2887	0.0869	0.0434	0.1505	0.3010	0.0869	0.1738
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2887	0.1443	0.0722	0.1443	0.0434	0.0217	0.0752	0.6019	0.1738	0.0869
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.2887	0.1443	0.0833	0.0251	0.0125	0.0434	0.3475	0.3475	0.1738
10	0.0104	0.0180	0.0361	0.0208	0.0104	0.0052	0.0722	0.1443	0.2887	0.0000	0.2500	0.1443	0.0125	0.0063	0.0217	0.1738	0.6019	0.3010
11	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.0722	0.1443	0.2500	0.0000	0.2887	0.0251	0.0125	0.0434	0.0869	0.3010	0.6019
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0833	0.1443	0.2887	0.0000	0.0502	0.0251	0.0869	0.1738	0.1738	0.3475
13	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0251	0.0125	0.0251	0.0502	0.0000	0.3623	0.1046	0.0523	0.0151	0.0302
14	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0217	0.0125	0.0063	0.0125	0.0251	0.3623	0.0000	0.2092	0.0261	0.0075	0.0151
15	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0752	0.0434	0.0217	0.0434	0.0869	0.1046	0.2092	0.0000	0.0906	0.0261	0.0523
16	0.0434	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3475	0.1738	0.0869	0.1738	0.0523	0.0261	0.0906	0.0000	0.2092	0.1046
17	0.0125	0.0217	0.0434	0.0251	0.0125	0.0063	0.0869	0.1738	0.3475	0.6019	0.3010	0.1738	0.0151	0.0075	0.0261	0.2092	0.0000	0.3623
18	0.0251	0.0434	0.0869	0.0502	0.0251	0.0125	0.1738	0.0869	0.1738	0.3010	0.6019	0.3475	0.0302	0.0151	0.0523	0.1046	0.3623	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2887	0.1443	0.0833	0.1443	0.2887	0.0722	0.0361	0.0208	0.0104	0.0208	0.0417	0.3475	0.0434	0.3475	0.1738	0.0251	0.0125
2	0.2887	0.0000	0.2500	0.1443	0.0722	0.1443	0.1250	0.0625	0.0361	0.0180	0.0361	0.0722	0.6019	0.0752	0.1738	0.0869	0.0434	0.0217
3	0.1443	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0722	0.0361	0.0722	0.1443	0.3010	0.1505	0.0869	0.1738	0.0869	0.0434
4	0.0833	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0417	0.0208	0.0417	0.0833	0.1738	0.0869	0.1738	0.3475	0.0502	0.0251
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0208	0.0104	0.0208	0.0417	0.0869	0.0434	0.3010	0.6019	0.0251	0.0125
6	0.2887	0.1443	0.0722	0.1443	0.2500	0.0000	0.0361	0.0180	0.0104	0.0052	0.0104	0.0208	0.1738	0.0217	0.6019	0.3010	0.0125	0.0063
7	0.0722	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1443	0.0722	0.1443	0.2887	0.1505	0.3010	0.0434	0.0869	0.1738	0.0869
8	0.0361	0.0625	0.1250	0.0722	0.0361	0.0180	0.2500	0.0000	0.2887	0.1443	0.0722	0.1443	0.0752	0.6019	0.0217	0.0434	0.0869	0.1738
9	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.2887	0.0000	0.2887	0.1443	0.0833	0.0434	0.3475	0.0125	0.0251	0.1738	0.3475
10	0.0104	0.0180	0.0361	0.0208	0.0104	0.0052	0.0722	0.1443	0.2887	0.0000	0.2500	0.1443	0.0217	0.1738	0.0063	0.0125	0.3010	0.6019
11	0.0208	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.0722	0.1443	0.2500	0.0000	0.2887	0.0434	0.0869	0.0125	0.0251	0.6019	0.3475
12	0.0417	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0833	0.1443	0.2887	0.0000	0.0722	0.1738	0.0251	0.0502	0.3475	0.1738
13	0.3475	0.6019	0.3010	0.1738	0.0869	0.1738	0.1505	0.0752	0.0434	0.0217	0.0434	0.0869	0.0000	0.0906	0.2092	0.1046	0.0523	0.0261
14	0.0434	0.0752	0.1505	0.0869	0.0434	0.0217	0.3010	0.6019	0.3475	0.1738	0.0869	0.1738	0.0906	0.0000	0.0261	0.0523	0.1046	0.2092
15	0.3475	0.1738	0.0869	0.1738	0.3010	0.6019	0.0434	0.0217	0.0125	0.0063	0.0125	0.0251	0.2092	0.0261	0.0000	0.3623	0.0151	0.0075
16	0.1738	0.0869	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0251	0.0125	0.0251	0.0502	0.1046	0.0523	0.3623	0.0000	0.0302	0.0151
17	0.0251	0.0434	0.0869	0.0502	0.0251	0.0125	0.1738	0.0869	0.1738	0.3475	0.6019	0.3475	0.0523	0.1046	0.0151	0.0302	0.0000	0.3623
18	0.0125	0.0217	0.0434	0.0251	0.0125	0.0063	0.0869	0.1738	0.3475	0.6019	0.3010	0.1738	0.0261	0.2092	0.0075	0.0151	0.3623	0.0000

2-2'-4-5-5'-6-HEXACHLOROBIPHENYL

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2887	0.1443	0.0722	0.1443	0.2887	0.0722	0.0361	0.0208	0.0120	0.0208	0.0417	0.3475	0.0869	0.1738	0.3475	0.0434	0.0251
2	0.2887	0.0000	0.2500	0.1250	0.0625	0.1443	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.6019	0.1505	0.0752	0.1738	0.0752	0.0434
3	0.1443	0.2500	0.0000	0.2500	0.1250	0.0625	0.2500	0.1250	0.0722	0.0417	0.0722	0.1443	0.3010	0.3010	0.1505	0.0752	0.1505	0.0869
4	0.0722	0.1250	0.2500	0.0000	0.2500	0.1250	0.1250	0.0625	0.0361	0.0208	0.0361	0.0722	0.1505	0.6019	0.3010	0.1505	0.0752	0.0434
5	0.1443	0.0722	0.1250	0.2500	0.0000	0.2500	0.0625	0.0313	0.0180	0.0104	0.0180	0.0361	0.0869	0.3010	0.6019	0.3010	0.0376	0.0217
6	0.2887	0.1443	0.0722	0.1250	0.2500	0.0000	0.0361	0.0180	0.0104	0.0060	0.0104	0.0208	0.1738	0.1505	0.3010	0.6019	0.0217	0.0125
7	0.0722	0.1250	0.2500	0.1250	0.0625	0.0313	0.0000	0.2500	0.1443	0.0833	0.1443	0.2887	0.1505	0.1505	0.0752	0.0376	0.3010	0.1738
8	0.0361	0.0625	0.1250	0.0625	0.0313	0.0156	0.2500	0.0000	0.2887	0.1667	0.0833	0.1443	0.0752	0.0752	0.0376	0.0188	0.6019	0.1003
9	0.0208	0.0361	0.0722	0.0361	0.0180	0.0090	0.1443	0.2887	0.0000	0.3333	0.1667	0.0962	0.0434	0.0434	0.0217	0.0109	0.3475	0.2006
10	0.0120	0.0208	0.0417	0.0208	0.0104	0.0052	0.0833	0.1667	0.3333	0.0000	0.2887	0.1667	0.0251	0.0251	0.0125	0.0063	0.2006	0.3475
11	0.0208	0.0361	0.0722	0.0361	0.0180	0.0090	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0434	0.0434	0.0217	0.0109	0.0869	0.6019
12	0.0417	0.0722	0.1443	0.0722	0.0361	0.0180	0.2887	0.1443	0.0833	0.1667	0.2887	0.0000	0.0869	0.0869	0.0434	0.0217	0.1738	0.3475
13	0.3475	0.6019	0.3010	0.1505	0.0752	0.1738	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.0000	0.1812	0.0906	0.2092	0.0906	0.0523
14	0.0869	0.1505	0.3010	0.6019	0.3010	0.1505	0.1505	0.0752	0.0434	0.0251	0.0434	0.0869	0.1812	0.0000	0.3623	0.1812	0.0906	0.0523
15	0.1738	0.0869	0.1505	0.3010	0.6019	0.3010	0.0752	0.0376	0.0217	0.0125	0.0217	0.0434	0.1046	0.3623	0.0000	0.3623	0.0453	0.0261
16	0.3475	0.1738	0.0869	0.1505	0.3010	0.6019	0.0434	0.0217	0.0125	0.0072	0.0125	0.0251	0.2092	0.1812	0.3623	0.0000	0.0261	0.0151
17	0.0434	0.0752	0.1505	0.0752	0.0376	0.0188	0.3010	0.6019	0.3475	0.2006	0.1003	0.1738	0.0906	0.0906	0.0453	0.0226	0.0000	0.1208
18	0.0251	0.0434	0.0869	0.0434	0.0217	0.0109	0.1738	0.0869	0.2006	0.3475	0.6019	0.3475	0.0523	0.0523	0.0261	0.0131	0.1046	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2500	0.1250	0.0722	0.1443	0.2500	0.0625	0.0313	0.0156	0.0078	0.0208	0.0361	0.3010	0.6019	0.3010	0.0376	0.0188	0.0094
2	0.2500	0.0000	0.2500	0.1443	0.0833	0.1250	0.1250	0.0625	0.0313	0.0156	0.0417	0.0722	0.1505	0.3010	0.6019	0.0752	0.0376	0.0188
3	0.1250	0.2500	0.0000	0.2887	0.1667	0.0833	0.2500	0.1250	0.0625	0.0313	0.0833	0.1443	0.1003	0.1505	0.3010	0.1505	0.0752	0.0376
4	0.0833	0.1443	0.2887	0.0000	0.3333	0.1667	0.1443	0.0722	0.0361	0.0180	0.0481	0.0833	0.2006	0.1003	0.1738	0.0869	0.0434	0.0217
5	0.1443	0.0722	0.1667	0.3333	0.0000	0.2887	0.0833	0.0417	0.0208	0.0104	0.0278	0.0481	0.3475	0.1738	0.0869	0.0502	0.0251	0.0125
6	0.2500	0.1250	0.0625	0.1667	0.2887	0.0000	0.0313	0.0156	0.0078	0.0039	0.0104	0.0180	0.6019	0.3010	0.1505	0.0188	0.0094	0.0047
7	0.0625	0.1250	0.2500	0.1443	0.0833	0.0417	0.0000	0.2500	0.1250	0.0625	0.1667	0.2887	0.0502	0.0752	0.1505	0.3010	0.1505	0.0752
8	0.0313	0.0625	0.1250	0.0722	0.0754	0.0208	0.2500	0.0000	0.2500	0.1250	0.0722	0.1443	0.0251	0.0376	0.0752	0.6019	0.3010	0.1505
9	0.0156	0.0313	0.0625	0.0361	0.0208	0.0104	0.1250	0.2500	0.0000	0.2500	0.1443	0.0833	0.0125	0.0188	0.0376	0.3010	0.6019	0.3010
10	0.0104	0.0208	0.0417	0.0241	0.0139	0.0069	0.0833	0.1250	0.2500	0.0000	0.2887	0.1667	0.0084	0.0125	0.0251	0.1505	0.3010	0.6019
11	0.0208	0.0417	0.0833	0.0481	0.0278	0.0139	0.1667	0.0833	0.1443	0.2887	0.0000	0.3333	0.0167	0.0251	0.0502	0.1003	0.1738	0.3475
12	0.0361	0.0722	0.1443	0.0833	0.0481	0.0241	0.2887	0.1443	0.0722	0.1667	0.3333	0.0000	0.0290	0.0434	0.0869	0.1738	0.0869	0.2006
13	0.3010	0.1505	0.0752	0.2006	0.3475	0.6019	0.0376	0.0188	0.0094	0.0047	0.0125	0.0217	0.0000	0.3623	0.1812	0.0226	0.0113	0.0057
14	0.6019	0.3010	0.1505	0.0869	0.1738	0.3010	0.0752	0.0376	0.0188	0.0094	0.0251	0.0434	0.3623	0.0000	0.3623	0.0453	0.0226	0.0113
15	0.3010	0.6019	0.3010	0.1738	0.1003	0.1505	0.1505	0.0752	0.0376	0.0188	0.0502	0.0869	0.1812	0.3623	0.0000	0.0906	0.0453	0.0226
16	0.0376	0.0752	0.1505	0.0869	0.0907	0.0251	0.3010	0.6019	0.3010	0.1505	0.0869	0.1738	0.0302	0.0453	0.0906	0.0000	0.3623	0.1812
17	0.0188	0.0376	0.0752	0.0434	0.0251	0.0125	0.1505	0.3010	0.6019	0.3010	0.1738	0.1003	0.0151	0.0226	0.0453	0.3623	0.0000	0.3623
18	0.0125	0.0251	0.0502	0.0290	0.0167	0.0084	0.1003	0.1505	0.3010	0.6019	0.3475	0.2006	0.0101	0.0151	0.0302	0.1812	0.3623	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.0000	0.2887	0.1443	0.0722	0.1667	0.2887	0.0722	0.0361	0.0208	0.0104	0.0241	0.0361	0.3475	0.0434	0.3475	0.0869	0.0434	0.0125
2	0.2887	0.0000	0.2500	0.1250	0.0722	0.1443	0.1250	0.0625	0.0361	0.0180	0.0361	0.0625	0.6019	0.0752	0.1738	0.1505	0.0752	0.0217
3	0.1443	0.2500	0.0000	0.2500	0.1443	0.0722	0.2500	0.1250	0.0722	0.0361	0.0722	0.1250	0.3010	0.1505	0.0869	0.3010	0.1505	0.0434
4	0.0833	0.1250	0.2500	0.0000	0.2887	0.1443	0.1250	0.0625	0.0361	0.0180	0.0361	0.0625	0.1505	0.0752	0.1738	0.6019	0.0752	0.0217
5	0.1667	0.0833	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0208	0.0104	0.0123	0.0361	0.1003	0.0434	0.3475	0.3475	0.0434	0.0125
6	0.2887	0.1443	0.0722	0.1443	0.2887	0.0000	0.0361	0.0180	0.0104	0.0052	0.0104	0.0180	0.1738	0.0217	0.6019	0.1738	0.0217	0.0063
7	0.0722	0.1250	0.2500	0.1250	0.0722	0.0361	0.0000	0.2500	0.1443	0.0722	0.1443	0.2500	0.1505	0.3010	0.0434	0.1505	0.3010	0.0869
8	0.0361	0.0625	0.1250	0.0625	0.0361	0.0180	0.2500	0.0000	0.2887	0.1443	0.0833	0.1250	0.0752	0.6019	0.0217	0.0752	0.1505	0.1738
9	0.0208	0.0361	0.0722	0.0361	0.0208	0.0104	0.1443	0.2887	0.0000	0.2887	0.1667	0.0833	0.0434	0.3475	0.0125	0.0434	0.1003	0.3475
10	0.0104	0.0180	0.0361	0.0180	0.0104	0.0052	0.0722	0.1443	0.2887	0.0000	0.2887	0.1443	0.0217	0.1738	0.0063	0.0069	0.1738	0.6019
11	0.0208	0.0361	0.0722	0.0361	0.0208	0.0104	0.1443	0.0722	0.1667	0.2887	0.0000	0.2887	0.0434	0.0869	0.0125	0.0434	0.3475	0.3475
12	0.0361	0.0625	0.1250	0.0625	0.0361	0.0180	0.2500	0.1250	0.0722	0.1443	0.2887	0.0000	0.0752	0.1505	0.0217	0.0752	0.6019	0.1738
13	0.3475	0.6019	0.3010	0.1505	0.0869	0.1738	0.1505	0.0752	0.0434	0.0217	0.0434	0.0752	0.0000	0.0906	0.2092	0.1812	0.0906	0.0261
14	0.0434	0.0752	0.1505	0.0752	0.0196	0.0217	0.3010	0.6019	0.3475	0.1738	0.1003	0.1505	0.0906	0.0000	0.0261	0.0906	0.1812	0.2092
15	0.3475	0.1738	0.0869	0.1738	0.3475	0.6019	0.0434	0.0217	0.0125	0.0063	0.0125	0.0217	0.2092	0.0261	0.0000	0.2092	0.0261	0.0075
16	0.1003	0.1505	0.3010	0.6019	0.3475	0.1738	0.1505	0.0752	0.0434	0.0217	0.0434	0.0752	0.1812	0.0906	0.2092	0.0000	0.0906	0.0261
17	0.0434	0.0752	0.1505	0.0752	0.0434	0.0217	0.3010	0.1505	0.0869	0.1738	0.3475	0.6019	0.0906	0.1812	0.0261	0.0906	0.0000	0.2092
18	0.0125	0.0217	0.0434	0.0217	0.0125	0.0063	0.0869	0.1738	0.3475	0.6019	0.3475	0.1738	0.0261	0.2092	0.0075	0.0026	0.2092	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	0.0000	0.2500	0.1250	0.0625	0.1443	0.2500	0.0625	0.0313	0.0156	0.0078	0.0208	0.0361	0.3010	0.6019	0.3010	0.0376	0.0188	0.0094	0.0752
2	0.2500	0.0000	0.2500	0.1250	0.0722	0.1250	0.1250	0.0625	0.0313	0.0156	0.0417	0.0722	0.1505	0.3010	0.6019	0.0752	0.0376	0.0188	0.1505
3	0.1250	0.2500	0.0000	0.2500	0.1443	0.0722	0.2500	0.1250	0.0625	0.0313	0.0833	0.1443	0.0869	0.1505	0.3010	0.1505	0.0752	0.0376	0.3010
4	0.0722	0.1250	0.2500	0.0000	0.2887	0.1443	0.1250	0.0625	0.0313	0.0156	0.0417	0.0722	0.1738	0.0869	0.1505	0.0752	0.0376	0.0188	0.6019
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0180	0.0090	0.0241	0.0417	0.3475	0.1738	0.0869	0.0434	0.0217	0.0109	0.3475
6	0.2500	0.1250	0.0625	0.1443	0.2887	0.0000	0.0313	0.0156	0.0078	0.0039	0.0104	0.0180	0.6019	0.3010	0.1505	0.0188	0.0094	0.0047	0.1738
7	0.0625	0.1250	0.2500	0.1250	0.0722	0.0361	0.0000	0.2500	0.1250	0.0625	0.1667	0.2887	0.0434	0.0752	0.1505	0.3010	0.1505	0.0752	0.1505
8	0.0313	0.0625	0.1250	0.0625	0.0361	0.0180	0.2500	0.0000	0.2500	0.1250	0.0722	0.1443	0.0217	0.0376	0.0752	0.6019	0.3010	0.1505	0.0752
9	0.0156	0.0313	0.0625	0.0313	0.0180	0.0090	0.1250	0.2500	0.0000	0.2500	0.1443	0.0833	0.0109	0.0188	0.0376	0.3010	0.6019	0.3010	0.0376
10	0.0104	0.0208	0.0417	0.0208	0.0120	0.0060	0.0833	0.1250	0.2500	0.0000	0.2887	0.1667	0.0072	0.0125	0.0251	0.1505	0.3010	0.6019	0.0251
11	0.0208	0.0417	0.0833	0.0417	0.0241	0.0120	0.1667	0.0833	0.1443	0.2887	0.0000	0.3333	0.0145	0.0251	0.0502	0.1003	0.1738	0.3475	0.0502
12	0.0361	0.0722	0.1443	0.0722	0.0417	0.0208	0.2887	0.1443	0.0722	0.1667	0.3333	0.0000	0.0251	0.0434	0.0869	0.1738	0.0869	0.2006	0.0869
13	0.3010	0.1505	0.0752	0.1738	0.3475	0.6019	0.0376	0.0188	0.0094	0.0047	0.0125	0.0217	0.0000	0.3623	0.1812	0.0226	0.0113	0.0057	0.2092
14	0.6019	0.3010	0.1505	0.0752	0.1738	0.3010	0.0752	0.0376	0.0188	0.0094	0.0251	0.0434	0.3623	0.0000	0.3623	0.0453	0.0226	0.0113	0.0906
15	0.3010	0.6019	0.3010	0.1505	0.0869	0.1505	0.1505	0.0752	0.0376	0.0188	0.0502	0.0869	0.1812	0.3623	0.0000	0.0906	0.0453	0.0226	0.1812
16	0.0376	0.0752	0.1505	0.0752	0.0434	0.0217	0.3010	0.6019	0.3010	0.1505	0.0869	0.1738	0.0261	0.0453	0.0906	0.0000	0.3623	0.1812	0.0906
17	0.0188	0.0376	0.0752	0.0376	0.0217	0.0109	0.1505	0.3010	0.6019	0.3010	0.1738	0.1003	0.0131	0.0226	0.0453	0.3623	0.0000	0.3623	0.0453
18	0.0125	0.0251	0.0502	0.0251	0.0145	0.0072	0.1003	0.1505	0.3010	0.6019	0.3475	0.2006	0.0087	0.0151	0.0302	0.1812	0.3623	0.0000	0.0302
19	0.0869	0.1505	0.3010	0.6019	0.3475	0.1738	0.1505	0.0752	0.0376	0.0188	0.0502	0.0869	0.2092	0.1046	0.1812	0.0906	0.0453	0.0226	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.0000	0.2500	0.1250	0.0625	0.1443	0.2887	0.0625	0.0313	0.0156	0.0090	0.0156	0.0313	0.6019	0.3010	0.1738	0.0752	0.0376	0.0188	0.0376	0.0188
2	0.2500	0.0000	0.2500	0.1250	0.0625	0.1443	0.1250	0.0625	0.0313	0.0180	0.0313	0.0625	0.3010	0.6019	0.0752	0.1505	0.0752	0.0376	0.0752	0.0376
3	0.1250	0.2500	0.0000	0.2500	0.1250	0.0722	0.2500	0.1250	0.0625	0.0361	0.0625	0.1250	0.1505	0.3010	0.1505	0.3010	0.1505	0.0752	0.1505	0.0752
4	0.0722	0.1250	0.2500	0.0000	0.2500	0.1443	0.1250	0.0625	0.0313	0.0180	0.0313	0.0625	0.0869	0.1505	0.3010	0.6019	0.0752	0.0376	0.0752	0.0376
5	0.1443	0.0722	0.1250	0.2500	0.0000	0.2887	0.0625	0.0313	0.0156	0.0090	0.0156	0.0313	0.1738	0.0869	0.6019	0.3010	0.0376	0.0188	0.0376	0.0188
6	0.2887	0.1443	0.0722	0.1443	0.2887	0.0000	0.0361	0.0180	0.0090	0.0052	0.0090	0.0180	0.3475	0.1738	0.3475	0.1738	0.0217	0.0109	0.0217	0.0109
7	0.0625	0.1250	0.2500	0.1250	0.0625	0.0361	0.0000	0.2500	0.1250	0.0722	0.1250	0.2500	0.0752	0.1505	0.0752	0.1505	0.3010	0.1505	0.3010	0.1505
8	0.0313	0.0625	0.1250	0.0625	0.0313	0.0180	0.2500	0.0000	0.2500	0.1443	0.0722	0.1250	0.0376	0.0752	0.0376	0.0752	0.6019	0.3010	0.1505	0.0869
9	0.0156	0.0313	0.0625	0.0313	0.0156	0.0090	0.1250	0.2500	0.0000	0.2887	0.1443	0.0722	0.0188	0.0376	0.0188	0.0376	0.3010	0.6019	0.0869	0.1738
10	0.0090	0.0180	0.0361	0.0180	0.0090	0.0052	0.0722	0.1443	0.2887	0.0000	0.2887	0.1443	0.0109	0.0217	0.0109	0.0217	0.1738	0.3475	0.1738	0.3475
11	0.0156	0.0313	0.0625	0.0313	0.0156	0.0090	0.1250	0.0625	0.1443	0.2887	0.0000	0.2500	0.0188	0.0376	0.0188	0.0376	0.0752	0.1738	0.3010	0.6019
12	0.0313	0.0625	0.1250	0.0625	0.0313	0.0180	0.2500	0.1250	0.0625	0.1443	0.2500	0.0000	0.0376	0.0752	0.0376	0.0752	0.1505	0.0752	0.6019	0.3010
13	0.6019	0.3010	0.1505	0.0752	0.1738	0.3475	0.0752	0.0376	0.0188	0.0109	0.0188	0.0376	0.0000	0.3623	0.2092	0.0906	0.0453	0.0226	0.0453	0.0226
14	0.3010	0.6019	0.3010	0.1505	0.0752	0.1738	0.1505	0.0752	0.0376	0.0217	0.0376	0.0752	0.3623	0.0000	0.0906	0.1812	0.0906	0.0453	0.0906	0.0453
15	0.1738	0.0869	0.1505	0.3010	0.6019	0.3475	0.0752	0.0376	0.0188	0.0109	0.0188	0.0376	0.2092	0.1046	0.0000	0.3623	0.0453	0.0226	0.0453	0.0226
16	0.0869	0.1505	0.3010	0.6019	0.3010	0.1738	0.1505	0.0752	0.0376	0.0217	0.0376	0.0752	0.1046	0.1812	0.3623	0.0000	0.0906	0.0453	0.0906	0.0453
17	0.0376	0.0752	0.1505	0.0752	0.0376	0.0217	0.3010	0.6019	0.3010	0.1738	0.0869	0.1505	0.0453	0.0906	0.0453	0.0906	0.0000	0.3623	0.1812	0.1046
18	0.0188	0.0376	0.0752	0.0376	0.0188	0.0109	0.1505	0.3010	0.6019	0.3475	0.1738	0.0869	0.0226	0.0453	0.0226	0.0453	0.3623	0.0000	0.1046	0.2092
19	0.0376	0.0752	0.1505	0.0752	0.0376	0.0217	0.3010	0.1505	0.0752	0.1738	0.3010	0.6019	0.0453	0.0906	0.0453	0.0906	0.1812	0.0906	0.0000	0.3623
20	0.0188	0.0376	0.0752	0.0376	0.0188	0.0109	0.1505	0.0752	0.1738	0.3475	0.6019	0.3010	0.0226	0.0453	0.0226	0.0453	0.0906	0.2092	0.3623	0.0000

1	0.0000	0.2500	0.1250	0.0625	0.1443	0.2500	0.0625	0.0313	0.0156	0.0090	0.0156	0.0313	0.6019	0.3010	0.3010	0.0752	0.0376	0.0188	0.0376	0.0188
2	0.2500	0.0000	0.2500	0.1250	0.0722	0.1250	0.1250	0.0625	0.0313	0.0180	0.0313	0.0625	0.3010	0.6019	0.1505	0.1505	0.0752	0.0376	0.0752	0.0376
3	0.1250	0.2500	0.0000	0.2500	0.1443	0.0722	0.2500	0.1250	0.0625	0.0361	0.0625	0.1250	0.1505	0.3010	0.0869	0.3010	0.1505	0.0752	0.1505	0.0752
4	0.0722	0.1250	0.2500	0.0000	0.2887	0.1443	0.1250	0.0625	0.0313	0.0180	0.0313	0.0625	0.0869	0.1505	0.1738	0.6019	0.0752	0.0376	0.0752	0.0376
5	0.1443	0.0722	0.1443	0.2887	0.0000	0.2887	0.0722	0.0361	0.0180	0.0104	0.0180	0.0361	0.1738	0.0869	0.3475	0.3475	0.0434	0.0217	0.0434	0.0217
6	0.2500	0.1250	0.0625	0.1443	0.2887	0.0000	0.0313	0.0156	0.0078	0.0045	0.0078	0.0156	0.3010	0.1505	0.6019	0.1738	0.0188	0.0094	0.0188	0.0094
7	0.0625	0.1250	0.2500	0.1250	0.0722	0.0361	0.0000	0.2500	0.1250	0.0722	0.1250	0.2500	0.0752	0.1505	0.0434	0.1505	0.3010	0.1505	0.3010	0.1505
8	0.0313	0.0625	0.1250	0.0625	0.0361	0.0180	0.2500	0.0000	0.2500	0.1443	0.0722	0.1250	0.0376	0.0752	0.0217	0.0752	0.6019	0.3010	0.1505	0.0869
9	0.0156	0.0313	0.0625	0.0313	0.0180	0.0090	0.1250	0.2500	0.0000	0.2887	0.1443	0.0722	0.0188	0.0376	0.0109	0.0376	0.3010	0.6019	0.0869	0.1738
10	0.0090	0.0180	0.0361	0.0180	0.0104	0.0052	0.0722	0.1443	0.2887	0.0000	0.2887	0.1443	0.0109	0.0217	0.0063	0.0217	0.1738	0.3475	0.1738	0.3475
11	0.0156	0.0313	0.0625	0.0313	0.0180	0.0090	0.1250	0.0625	0.1443	0.2887	0.0000	0.2500	0.0188	0.0376	0.0109	0.0376	0.0752	0.1738	0.3010	0.6019
12	0.0313	0.0625	0.1250	0.0625	0.0361	0.0180	0.2500	0.1250	0.0625	0.1443	0.2500	0.0000	0.0376	0.0752	0.0217	0.0752	0.1505	0.0752	0.6019	0.3010
13	0.6019	0.3010	0.1505	0.0752	0.1738	0.3010	0.0752	0.0376	0.0188	0.0109	0.0188	0.0376	0.0000	0.3623	0.3623	0.0906	0.0453	0.0226	0.0453	0.0226
14	0.3010	0.6019	0.3010	0.1505	0.0869	0.1505	0.1505	0.0752	0.0376	0.0217	0.0376	0.0752	0.3623	0.0000	0.1812	0.1812	0.0906	0.0453	0.0906	0.0453
15	0.3010	0.1505	0.0752	0.1738	0.3475	0.6019	0.0376	0.0188	0.0094	0.0054	0.0094	0.0188	0.3623	0.1812	0.0000	0.2092	0.0226	0.0113	0.0226	0.0113
16	0.0869	0.1505	0.3010	0.6019	0.3475	0.1738	0.1505	0.0752	0.0376	0.0217	0.0376	0.0752	0.1046	0.1812	0.2092	0.0000	0.0906	0.0453	0.0906	0.0453
17	0.0376	0.0752	0.1505	0.0752	0.0434	0.0217	0.3010	0.6019	0.3010	0.1738	0.0869	0.1505	0.0453	0.0906	0.0261	0.0906	0.0000	0.3623	0.1812	0.1046
18	0.0188	0.0376	0.0752	0.0376	0.0217	0.0109	0.1505	0.3010	0.6019	0.3475	0.1738	0.0869	0.0226	0.0453	0.0131	0.0453	0.3623	0.0000	0.1046	0.2092
19	0.0376	0.0752	0.1505	0.0752	0.0434	0.0217	0.3010	0.1505	0.0752	0.1738	0.3010	0.6019	0.0453	0.0906	0.0261	0.0906	0.1812	0.0906	0.0000	0.3623
20	0.0188	0.0376	0.0752	0.0376	0.0217	0.0109	0.1505	0.0752	0.1738	0.3475	0.6019	0.3010	0.0226	0.0453	0.0453	0.0453	0.0906	0.2092	0.3623	0.0000

1	0.0000	0.2500	0.1250	0.0722	0.1250	0.2500	0.0625	0.0313	0.0156	0.0078	0.0180	0.0361	0.6019	0.3010	0.3010	0.1505	0.0376	0.0188	0.0094	0.0217
2	0.2500	0.0000	0.2500	0.1443	0.0722	0.1250	0.1250	0.0625	0.0313	0.0156	0.0361	0.0722	0.3010	0.6019	0.1505	0.0869	0.0752	0.0376	0.0188	0.0434
3	0.1250	0.2500	0.0000	0.2887	0.1443	0.0722	0.2500	0.1250	0.0625	0.0313	0.0722	0.1443	0.1505	0.3010	0.0869	0.1738	0.1505	0.0752	0.0376	0.0869
4	0.0722	0.1443	0.2887	0.0000	0.2887	0.1443	0.1443	0.0722	0.0361	0.0180	0.0417	0.0833	0.0869	0.1738	0.1738	0.3475	0.0869	0.0434	0.0217	0.0502
5	0.1250	0.0625	0.1443	0.2887	0.0000	0.2500	0.0722	0.0361	0.0180	0.0090	0.0208	0.0417	0.1505	0.0752	0.3010	0.6019	0.0434	0.0217	0.0109	0.0251
6	0.2500	0.1250	0.0625	0.1443	0.2500	0.0000	0.0313	0.0156	0.0078	0.0039	0.0090	0.0180	0.3010	0.1505	0.6019	0.3010	0.0188	0.0094	0.0047	0.0109
7	0.0625	0.1250	0.2500	0.1443	0.0722	0.0361	0.0000	0.2500	0.1250	0.0625	0.1443	0.2887	0.0752	0.1505	0.0434	0.0869	0.3010	0.1505	0.0752	0.1738
8	0.0313	0.0625	0.1250	0.2500	0.0361	0.0180	0.2500	0.0000	0.2500	0.1250	0.0625	0.1443	0.0376	0.0752	0.0217	0.0434	0.6019	0.3010	0.1505	0.0752
9	0.0156	0.0313	0.0625	0.0361	0.0180	0.0090	0.1250	0.2500	0.0000	0.2500	0.1250	0.0722	0.0188	0.0376	0.0109	0.0217	0.3010	0.6019	0.3010	0.1505
10	0.0090	0.0180	0.0361	0.0208	0.0104	0.0052	0.0722	0.1250	0.2500	0.0000	0.2500	0.1443	0.0109	0.0217	0.0063	0.0125	0.1505	0.3010	0.6019	0.3010
11	0.0180	0.0361	0.0722	0.0417	0.0208	0.0104	0.1443	0.0722	0.1250	0.2500	0.0000	0.2887	0.0217	0.0434	0.0125	0.0251	0.0869	0.1505	0.3010	0.6019
12	0.0361	0.0722	0.1443	0.0833	0.0417	0.0208	0.2887	0.1443	0.0722	0.1443	0.2887	0.0000	0.0434	0.0869	0.0251	0.0502	0.1738	0.0869	0.1738	0.3475
13	0.6019	0.3010	0.1505	0.0869	0.1505	0.3010	0.0752	0.0376	0.0188	0.0094	0.0217	0.0434	0.0000	0.3623	0.3623	0.1812	0.0453	0.0226	0.0113	0.0261
14	0.3010	0.6019	0.3010	0.1738	0.0869	0.1505	0.1505	0.0752	0.0376	0.0188	0.0434	0.0869	0.3010	0.0000	0.1812	0.1046	0.0906	0.0453	0.0226	0.0523
15	0.3010	0.1505	0.0752	0.1738	0.3010	0.6019	0.0376	0.0188	0.0094	0.0047	0.0109	0.0217	0.3623	0.1812	0.0000	0.3623	0.0226	0.0113	0.0057	0.0131
16	0.1505	0.0752	0.1738	0.3475	0.6019	0.3010	0.0869	0.0434	0.0217	0.0109	0.0251	0.0502	0.1812	0.0906	0.3623	0.0000	0.0523	0.0261	0.0131	0.0302
17	0.0376	0.0752	0.1505	0.3010	0.0434	0.0217	0.3010	0.6019	0.3010	0.1505	0.0752	0.1738	0.0453	0.0906	0.0261	0.0523	0.0000	0.3623	0.1812	0.0906
18	0.0188	0.0376	0.0752	0.0434	0.0217	0.0109	0.1505	0.3010	0.6019	0.3010	0.1505	0.0869	0.0226	0.0453	0.0131	0.0261	0.3623	0.0000	0.3623	0.1812
19	0.0109	0.0217	0.0434	0.0251	0.0125	0.0063	0.0869	0.1505	0.3010	0.6019	0.3010	0.1738	0.0131	0.0261	0.0075	0.0151	0.1812	0.3623	0.0000	0.3623
20	0.0217	0.0434	0.0869	0.0502	0.0251	0.0125	0.1738	0.0869	0.1505	0.3010	0.6019	0.3475	0.0261	0.0523	0.0151	0.0302	0.1046	0.1812	0.3623	0.0000

APPENDIX II

CHARACTERISTIC POLYNOMIALS OF PCB CONGENERS

BIPHENYL

$$x^{12} - 1.9049x^{10} - 1.1492x^{9} + 0.4376x^{8} + 0.6520x^{7} + 0.2333x^{6} + 0.0245x^{5} - 0.0035x^{4} - 0.0007x^{3}$$

2-CHLORO BIPHENYL

$$x^{13} - 2.4252x^{11} - 1.6485x^{10} + 0.7260x^{9} + 1.2136x^{8} + 0.4745x^{7} + 0.0304x^{6} - 0.0266x^{5} - 0.0067x^{4} - 0.0003x^{3} + 0.0001x^{2}$$

4-CHLORO BIPHENYL

$$x^{13} - 2.5138x^{11} - 1.6581x^{10} + 0.9514x^{9} + 1.4692x^{8} 0.5862x^{7} + 0.0470x^{6} - 0.0285x^{5} - 0.0073x^{4} - 0.0002x^{3} + 0.0001x^{2}$$

2-2'- DICHLORO BIPHENYL

$$x^{14} - 3.1286x^{12} - 2.2895x^{11} + 1.4719x^{10} + 2.4290x^{9} + 0.9294x^{8} - 0.0540x^{7} - 0.1226x^{6} - 0.0222x^{5} + 0.0032x^{4} + 0.0013x^{3}$$

4-4' DICHLORO BIPHENYL

$$x^{14} - 3.0725x^{12} - 2.1138x^{11} + 1.7620x^{10} + 2.7446x^{9} + 1.1412x^{8} + 0.0110x^{7} - 0.1344x^{6} - 0.0400x^{5} - 0.0030x^{4} + 0.0004x^{3}$$

2-5- DICHLORO BIPHENYL

$$x^{14} - 3.1288x^{12} - 2.2679x^{11} + 1.4982x^{10} + 2.3660x^{9} + 0.7529x^{8} - 0.2403x^{7} - 0.2306x^{6} - 0.0585x^{5} - 0.0032x^{4} + 0.0010x^{3} + 0.0001x^{2}$$

2-6- DICHLORO BIPHENYL

$$x^{14} - 3.1374x^{12} - 2.3386x^{11} + 1.3401x^{10} + 2.2198x^{9} + 0.7182x^{8} - 0.1949x^{7} - 0.1850x^{6} - 0.0400x^{5} + 0.0004x^{4} + 0.0012x^{3} + 0.0001x^{2}$$

2-4' DICHLORO BIPHENYL

$$x^{14} - 3.1252x^{12} - 2.2261x^{11} + 1.6578x^{10} + 2.6705x^{9} + 1.0945x^{8} + 0.0016x^{7} - 0.1206x^{6} - 0.0274x^{5} + 0.0016x^{4} + 0.0012x^{3} + 0.0001x^{2}$$

3-4- DICHLORO BIPHENYL

$$x^{14} - 3.2059x^{12} - 2.4582x^{11} + 1.4148x^{10} + 2.5923x^{9} + 1.1437x^{8} + 0.0522x^{7}$$
$$-0.1070x^{6} - 0.0287x^{5} + 0.0003x^{4} + 0.0010x^{3} + 0.0001x^{2}$$

3-3'- DICHLORO BIPHENYL

$$x^{14} - 3.1250x^{12} - 2.2014x^{11} + 1.7252x^{10} + 2.7363x^{9} + 1.1109x^{8} - 0.0159x^{7}$$
$$-0.1360x^{6} - 0.0320x^{5} + 0.0014x^{4} + 0.0013x^{3} + 0.0001x^{2}$$

2-2'-3- TRICHLORO BIPHENYL

$$x^{15} - 3.7947x^{13} - 3.0270x^{12} + 2.3471x^{11} + 4.2117x^{10} + 1.7857x^{9} - 0.1587x^{8}$$
$$-0.3350x^{7} - 0.0698x^{6} + 0.0133x^{5} + 0.0065x^{4} + 0.0003x^{3} - 0.0002x^{2}$$

2-2'-4- TRICHLORO BIPHENYL

$$x^{15} - 3.7579x^{13} - 2.9013x^{12} + 2.4872x^{11} + 4.2032x^{10} + 1.6175x^{9} - 0.3355x^{8}$$
$$-0.4214x^{7} - 0.0874x^{6} + 0.0154x^{5} + 0.0084x^{4} + 0.0007x^{3} - 0.0001x^{2}$$

2-2'-5- TRICHLORO BIPHENYL

$$x^{15} - 3.7439x^{13} - 2.8626x^{12} + 2.4898x^{11} + 4.0774x^{10} + 1.3854x^{9} - 0.5463x^{8}$$
$$-0.5315x^{7} - 0.1183x^{6} + 0.0137x^{5} + 0.0101x^{4} + 0.0013x^{3} - 0.0001x^{2}$$

2-3-4'- TRICHLORO BIPHENYL

$$x^{15} - 3.7959x^{13} - 2.9736x^{12} + 2.5537x^{11} + 4.5274x^{10} + 2.0216x^{9} - 0.0911x^{8}$$
$$-0.3585x^{7} - 0.0959x^{6} + 0.0054x^{5} + 0.0062x^{4} + 0.0008x^{3}$$

2-4'-5- TRICHLORO BIPHENYL

$$x^{15} - 3.7426x^{13} - 2.7992x^{12} + 2.7064x^{11} + 4.3822x^{10} + 1.5848x^{9} - 0.5205x^{8}$$
$$-0.5836x^{7} - 0.1572x^{6} + 0.0018x^{5} + 0.0091x^{4} + 0.0016x^{3} + 0.0001x^{2}$$

2-3-3'- TRICHLORO BIPHENYL

$$x^{15} - 3.7935x^{13} - 2.9803x^{12} + 2.5001x^{11} + 4.4184x^{10} + 1.9161x^{9} - 0.1389x^{8}$$
$$-0.3589x^{7} - 0.0853x^{6} + 0.0103x^{5} + 0.0069x^{4} + 0.0006x^{3} - 0.0001x^{2}$$

3-4-4'- TRICHLORO BIPHENYL

$$x^{15} - 3.7937x^{13} - 2.9208x^{12} + 2.7162x^{11} + 4.7336x^{10} + 2.1343x^{9} - 0.0949x^{8}$$
$$-0.3982x^{7} - 0.1174x^{6} + 0.0011x^{5} + 0.0066x^{4} + 0.0011x^{3}$$

2-4-4'-TRICHLORO BIPHENYL

$$x^{15} - 3.7596x^{13} - 2.8592x^{12} + 2.6514x^{11} + 4.4445x^{10} + 1.7779x^{9} - 0.3168x^{8}$$
$$-0.4669x^{7} - 0.1210x^{6} + 0.0054x^{5} + 0.0077x^{4} + 0.0011x^{3}$$

2-4-5- TRICHLORO BIPHENYL

$$x^{15} - 3.8338x^{13} - 3.1212x^{12} + 2.2201x^{11} + 3.9912x^{10} + 1.4306x^{9} - 0.5179x^{8}$$
$$-0.5503x^{7} - 0.1415x^{6} + 0.0051x^{5} + 0.0094x^{4} + 0.0017x^{3} + 0.0001x^{2}$$

2-4-6- TRICHLORO BIPHENYL

$$x^{15} - 3.8182x^{13} - 3.0917x^{12} + 2.1669x^{11} + 3.7949x^{10} + 1.2261x^{9} - 0.5823x^{8}$$
$$-0.5046x^{7} - 0.0880x^{6} + 0.0280x^{5} + 0.0142x^{4} + 0.0021x^{3}$$

2-2'-3-4- TETRACHLORO BIPHENYL

$$x^{16} - 4.4823x^{14} - 3.8709x^{13} + 3.4228x^{12} + 6.6002x^{11} + 2.8880x^{10} - 0.6267x^{9}$$
$$-0.9455x^{8} - 0.2380x^{7} + 0.0409x^{6} + 0.0304x^{5} + 0.0038x^{4} - 0.0006x^{3}$$
$$-0.0002x^{2}$$

2-2'-3-5'- TETRACHLORO BIPHENYL

$$x^{16} - 4.4148x^{14} - 3.6187x^{13} + 3.7473x^{12} + 6.6533x^{11} + 2.5809x^{10} - 0.9986x^{9}$$
$$-1.1350x^{8} - 0.2686x^{7} + 0.548x^{6} + 0.0382x^{5} + 0.0049x^{4} - 0.0008x^{3}$$
$$-0.0003x^{2}$$

2-2'-4-4'- TETRACHLORO BIPHENYL

$$x^{16} - 4.4046x^{14} - 3.5604x^{13} + 3.8832x^{12} + 6.8231x^{11} + 2.7065x^{10} - 0.9384x^{9}$$
$$-1.1102x^{8} - 0.2559x^{7} + 0.0610x^{6} + 0.0401x^{5} + 0.0052x^{4} - 0.0007x^{3}$$
$$-0.0002x^{2}$$

3-3′-4-4′- TETRACHLORO BIPHENYL

$$x^{16} - 4.4642x^{14} - 3.6743x^{13} + 4.0368x^{12} + 7.5242x^{11} + 3.6461x^{10} - 0.3093x^{9}$$
$$-0.9231x^{8} - 0.2783x^{7} + 0.0233x^{6} + 0.0284x^{5} + 0.0043x^{4} - 0.0005x^{3}$$
$$-0.0002x^{2}$$

2-3-5-6- TETRACHLORO BIPHENYL

$$x^{16} - 4.4896x^{14} - 4.0123x^{13} + 2.8935x^{12} + 5.6344x^{11} + 1.8219x^{10} - 1.3957x^{9}$$
$$-1.3042x^{8} - 0.3259x^{7} + 0.0499x^{6} + 0.0475x^{5} + 0.0109x^{4} + 0.0010x^{3}$$

2-4-4′-5- TETRACHLORO BIPHENYL

$$x^{16} - 4.4330x^{14} - 3.6377x^{13} + 3.8243x^{12} + 6.8206x^{11} + 2.6561x^{10} - 1.1076x^{9}$$
$$-1.3072x^{8} - 0.3705x^{7} + 0.0295x^{6} + 0.0413x^{5} + 0.0090x^{4} + 0.0005x^{3}$$
$$-0.0001x^{2}$$

2-3-4-5- TETRACHLORO BIPHENYL

$$x^{16} - 4.5631x^{14} - 4.1822x^{13} + 2.8943x^{12} + 6.0318x^{11} + 2.3732x^{10} - 1.0701x^{9}$$
$$-1.2539x^{8} - 0.3762x^{7} + 0.0143x^{6} + 0.0374x^{5} + 0.0097x^{4} + 0.0010x^{3}$$

2-2′-5-6′- TETRACHLORO BIPHENYL

$$x^{16} - 4.3658x^{14} - 3.5256x^{13} + 3.6316x^{12} + 6.1274x^{11} + 1.9100x^{10} - 1.3946x^{9}$$
$$-1.1909x^{8} - 0.1927x^{7} + 1.1111x^{6} + 0.0561x^{5} + 0.0075x^{4} - 0.0008x^{3}$$
$$-0.0003x^{2}$$

2-2′-4-5- TETRACHLORO BIPHENYL

$$x^{16} - 4.4363x^{14} - 3.7104x^{13} + 3.5822x^{12} + 6.4895x^{11} + 2.4802x^{10} - 1.0453x^{9}$$
$$-1.1590x^{8} - 0.2820x^{7} + 0.0497x^{6} + 0.00374x^{5} + 0.0050x^{4} - 0.0007x^{3}$$
$$-0.0003x^{2}$$

2-3′-4-4′-5- PENTACHLORO BIPHENYL

$$x^{17} - 5.1048x^{15} - 4.4016x^{14} + 5.5310x^{13} + 10.4547x^{12} + 4774x^{11} - 1.9386x^{10}$$
$$-2.5192x^{9} - 0.7211x^{8} + 0.1321x^{7} + 0.1277x^{6} + 0.0237x^{5} - 0.0023x^{4}$$
$$-0.0014x^{3} - 0.0002x^{2}$$

2-3-4-4'- TETRACHLOROBIPHENYL

$$x^{16} - 4.4792x^{14} - 3.7988x^{13} + 3.6660x^{12} + 6.9402x^{11} + 3.0845x^{10} - 0.6627x^{9}$$
$$- 1.0726x^{8} - 0.3177x^{7} + 0.0218x^{6} + 0.0333x^{5} + 0.0071x^{4} + 0.0004x^{3}$$

2-2'-5-5'- TETRACHOLORO BIPHENYL

$$x^{16} - 4.3627x^{14} - 3.4498x^{13} + 3.8603x^{12} + 6.3797x^{11} + 1.9513x^{10} - 1.5572x^{9}$$
$$- 1.3516x^{8} - 0.2458x^{7} + 0.1214x^{6} + 0.0714x^{5} + 0.0132x^{4} + 0.0002x^{3}$$
$$- 0.0003x^{2}$$

2-3'-4-4'- TETRACHLORO BIPHENYL

$$x^{16} - 4.3865x^{14} - 3.5005x^{13} + 0.9739x^{12} + 6.9200x^{11} + 2.7932x^{10} - 0.8852x^{9}$$
$$- 1.1014x^{8} - 0.2705x^{7} + 0.0480x^{6} 0.0352x^{5} + 0.0043x^{4} - 0.0008x^{3}$$
$$- 0.0002x^{2}$$

2-3'-4'-5- TETRACHLORO BIPHENYL

$$x^{16} - 4.4766x^{14} - 3.9356x^{13} + 3.0922x^{12} + 6.0063x^{11} + 2.4021x^{10} - 0.7129x^{9}$$
$$- 0.7627x^{8} - 0.0624x^{7} + 0.1105x^{6} + 0.0398x^{5} + 0.0011x^{4} - 0.0019x^{3}$$
$$- 0.0004x^{2}$$

2-2'-3-3'- TETRACHLORO BIPHENYL

$$x^{16} - 4.4656x^{14} - 3.7828x^{13} + 3.6413x^{12} + 6.9394x^{11} + 3.2517x^{10} - 0.3536x^{9}$$
$$- 0.8096x^{8} - 0.2022x^{7} + 0.0385x^{6} + 0.0249x^{5} + 0.0021x^{4} - 0.0008x^{3}$$
$$- 0.0002x^{2}$$

2-2'-6-6'- TETRACHLORO BIPHENYL

$$x^{16} - 4.4262x^{14} - 3.8303x^{13} + 3.0885x^{12} + 5.7794x^{11} + 2.0526x^{10} - 1.0360x^{9}$$
$$- 0.9861x^{8} - 0.1739x^{7} + 0.0788x^{6} + 0.0397x^{5} + 0.0046x^{4} - 0.0007x^{3}$$
$$- 0.0002x^{2}$$

2-3-3'-4-4'- PENTACHLORO BIPHENYL

$$x^{17} - 5.0684x^{15} - 4.4025x^{14} + 5.2505x^{13} + 9.9517x^{12} + 4.2071x^{11} - 1.7796x^{10}$$
$$-2.2101x^{9} - 0.5379x^{8} + 0.1763x^{7} + 0.1233x^{6} + 0.0180x^{5} - 0.0037x^{4}$$
$$-0.0016x^{x3} - 0.0002x^{2}$$

2-3-4-5-6- PENTACHLORO BIPHENYL

$$x^{17} - 5.2923x^{15} - 5.2528x^{14} + 3.9661x^{13} + 8.9606x^{12} + 3.6394x^{11} - 2.3649x^{10}$$
$$-2.8597x^{9} - 0.9358x^{8} + 0.0992x^{7} + 0.1781x^{6} + 0.0635x^{5} + 0.0117x^{4}$$
$$+0.0012x^{3} + 0.0001x^{2}$$

2-2'-3-4-4'- PENTACHLORO BIPHENYL

$$x^{17} - 5.1171x^{15} - 5.5029x^{14} + 5.2709x^{13} + 10.1869x^{12} + 4.4724x^{11} - 1.6708x^{10}$$
$$-2.2289x^{9} - 0.5765x^{8} + 0.1605x^{7} + 0.1218x^{6} + 0.0191x^{5} - 0.0032x^{4}$$
$$-0.0015x^{3} - 0.0002x^{2}$$

2-2'-3-5'-6- PENTACHLORO BIPHENYL

$$x^{17} - 5.0526x^{15} - 4.3486x^{14} + 5.1443x^{13} + 9.2871x^{12} + 3.0453x^{11} - 2.7681x^{10}$$
$$-2.5727x^{9} - 0.4643x^{8} + 0.3166x^{7} + 0.1863x^{6} + 0.0293x^{5} - 0.0046x^{4}$$
$$-0.0024x^{3} - 0.0003x^{2}$$

2-2'-4-6-6'- PENTACHLORO BIPHENYL

$$x^{17} - 5.0429x^{15} - 4.3765x^{14} + 4.9629x^{13} + 9.0359x^{12} + 3.0491x^{11} - 2.4158x^{10}$$
$$-2.1736x^{9} - 0.2823x^{8} + 0.3136x^{7} + 0.1409x^{6} + 0.0061x^{5} - 0.0097x^{4}$$
$$-0.0026x^{3} - 0.0002x^{2}$$

2-2'-3-4-5'- PENTACHLORO BIPHENYL

$$x^{17} - 5.1022x^{15} - 4.4629x^{14} + 5.2400x^{13} + 9.9227x^{12} + 4.0026x^{11} - 2.0876x^{10}$$
$$-2.4068x^{9} - 0.5696x^{8} + 0.2112x^{7} + 0.1486x^{6} + 0.0247x^{5} - 0.0036x^{4}$$
$$-0.0020x^{3} - 0.0003x^{2}$$

2-2′-4-4′-5- PENTACHLORO BIPHENYL

$$x^{17} - 5.0700x^{15} - 4.3390x^{14} + 5.3998x^{13} + 9.9299x^{12} + 3.8017x^{11} - 2.3226x^{10}$$
$$-2.5227x^{9} - 0.5845x^{8} + 0.2203x^{7} + 0.1512x^{6} + 0.0239x^{5} - 0.0039x^{4}$$
$$-0.0019x^{3} - 0.0002x^{2}$$

2-2′-4-5-5′- PENTACHLORO BIPHENYL

$$x^{17} - 5.0564x^{15} - 4.3039x^{14} + 5.3676x^{13} + 9.6846x^{12} + 3.3765x^{11} - 2.6826x^{10}$$
$$-2.6477x^{9} - 0.5376x^{8} + 0.2950x^{7} + 0.1884x^{6} + 0.0324x^{5} - 0.0040x^{4}$$
$$-0.0025x^{3} - 0.0004x^{2}$$

2-3-3′-4′-6- PENTACHLORO BIPHENYL

$$x^{17} - 5.0982x^{15} - 4.4291x^{14} + 5.3525x^{13} + 10.1208x^{12} + 4.1949x^{11} - 2.0137x^{10}$$
$$-2.4619x^{9} - 0.6689x^{8} + 0.1421x^{7} + 0.1221x^{6} + 0.0202x^{5} - 0.0029x^{4}$$
$$-0.0014x^{3} - 0.0001x^{2}$$

2-2′-3-3′-6-6′- HEXACHLORO BIPHENYL

$$x^{18} - 5.7436x^{16} - 5.2625x^{15} + 6.8187x^{14} + 13.1580x^{13} + 4.5924x^{12} - 4.6642x^{11}$$
$$-4.6221x^{10} - 0.8258x^{9} + 0.7442x^{8} + 8.4467x^{7} + 0.0608x^{6} - 0.0231x^{5}$$
$$-0.0100x^{4} - 0.0012x^{3} + 0.0001x^{2}$$

2-2′-3-4-4′-5- HEXACHLORO BIPHENYL

$$x^{18} - 5.7342x^{16} - 5.2825x^{15} + 6.7926x^{14} + 13.4268x^{12} - 3.9863x^{11} - 4.4613x^{10}$$
$$-1.0423x^{9} + 0.5432x^{8} + 0.3913x^{7} + 0.0719x^{6} - 0.0116x^{5} - 0.0074x^{4}$$
$$-0.0012x^{3} - 0.0001x^{2}$$

2-2′-3-4-5-5′- HEXACHLORO BIPHENYL

$$x^{18} - 5.7978x^{16} - 5.3791x^{15} + 6.9305x^{14} + 13.7355x^{13} + 5.2194x^{12} - 4.5796x^{11}$$
$$-4.9976x^{10} - 1.1565x^{9} + 0.6685x^{8} + 0.4950x^{7} + 0.0994x^{6} - 0.01444x^{5}$$
$$-0.0113x^{4} - 0.0024x^{3} - 0.0002x^{2}$$

2-2′-3-4′-5-5′- HEXACHLORO BIPHENYL

$$x^{18} - 5.7510x^{16} - 5.1768x^{15} + 20.2660x^{14} + 13.9654x^{13} + 5.2230x^{12} - 4.6231x^{11}$$
$$-4.9298x^{10} - 1.0461x^{9} + 0.7159x^{8} + 0.4856x^{7} + 0.0828x^{6} - 0.0202x^{5}$$
$$-0.0114x^{4} - 0.0019x^{3} - 0.0001x^{2}$$

2-2′-4-6′-5-5′- HEXACHLORO BIPHENYL

$$x^{18} - 5.7490x^{16} - 5.1541x^{15} + 7.3525x^{14} + 14.1306x^{13} + 5.3935x^{12} - 4.5495x^{11}$$
$$-4.9672x^{10} - 1.1213x^{9} + 0.6664x^{8} + 0.4699x^{7} + 0.0825x^{6} - 0.0183x^{5}$$
$$-0.0106x^{4} - 0.0017x^{3}$$

2-2′-4-5-5′-6- HEXACHLORO BIPHENYL

$$x^{18} - 5.7631x^{16} - 5.3054x^{15} + 6.8325x^{14} + 13.2582x^{13} + 4.6300x^{12} - 4.7833x^{11}$$
$$-4.7616x^{10} - 0.8447x^{9} + 0.8080x^{8} + 0.4963x^{7} + 0.0707x^{6} - 0.0294x^{5}$$
$$-0.0152x^{4} - 0.0029x^{3} - 0.0003x^{2}$$

2-2′-3-3′-4-4′ HEXACHLORO BIPHENYL

$$x^{18} - 5.8438x^{16} - 5.4831x^{15} + 7.1530x^{14} + 14.9279x^{13} + 7.2901x^{12} - 2.7128x^{11}$$
$$-4.2037x^{10} - 1.2507x^{9} + 0.3540x^{8} + 0.3218x^{7} + 0.0606x^{6} - 0.0109x^{5}$$
$$-0.0065x^{4} - 0.0010x^{3}$$

2-2′-4-4′-5-5′- HEXACHLORO BIPHENYL

$$x^{18} - 5.7757x^{16} - 5.1988 - x^{15} + 7.4198x^{14} + 14.3507x^{13} + 5.5595x^{12} - 4.5905x^{11}$$
$$-5.1020x^{10} - 1.1944x^{9} + 0.6660x^{8} + 0.4862x^{7} + 0.0897x^{6} - 0.0174x^{5}$$
$$-0.0108x^{4} - 0.0018x^{3} - 0.0001x^{2}$$

2-2′-4-4′-6-6′- HEXACHLORO BIPHENYL

$$x^{18} - 5.7003x^{16} - 5.7003x^{16} - 5.1190x^{15} + 6.9399x^{14} + 13.0650x^{13} + 4.4455x^{12}$$
$$-4.5066x^{11} - 4.1913x^{10} - 0.4878x^{9} + 0.8182x^{8} + 0.3825x^{7} + 0.0040x^{6}$$
$$-0.0412x^{5} - 0.0112x^{4} - 0.0002x^{3} + 0.0004x^{2} + 0.0001x^{1}$$

2-2′-3-3′-4-4′-6 HEPTACHLORO BIPHENYL

$$x^{19} - 6.5015x^{17} - 6.3167x^{16} + 6.2225x^{15} + 19.4387x^{14} + 8.4317x^{13} - 6.6077x^{12}$$
$$-8.1746x^{11} - 2.0413x^{10} + 1.2821x^{9} + 0.9835x^{8} + 0.1725x^{7} - 0.0599x^{6}$$
$$-0.0343x^{5} - 0.0058x^{4} + 0.0001x^{2}$$

2-2′-3-3′-4-4′-5-5′-OCTACHLORO BIPHENYL

$$x^{20} - 7.2420x^{18} - 7.3730x^{17} + 11.8998x^{16} + 26.3744x^{15} + 11.7480x^{14} - 11.4455x^{13}$$
$$-14.9330x^{12} - 4.1491x^{11} + 2.8646x^{10} + 2.5957x^{9} + 0.6274x^{8} - 0.1438x^{7}$$
$$-0.1347x^{6} - 0.0377x^{5} - 0.0047x^{4} + 0.0001x^{2}$$

2-2′-3-3′-4-5′-6-6′ OCTACHLORO BIPHENYL

$$x^{20} - 7.1654x^{18} - 7.2012x^{17} + 11.5070x^{16} + 24.4499x^{15} + 8.9208x^{14} - 12.9418x^{13}$$
$$-14.1406x^{12} - 2.5212x^{11} + 3.7019x^{10} + 2.5319x^{9} + 8.3389x^{8} - 0.2849x^{7}$$
$$-0.1517x^{6} - 0.0256x^{5} + 0.0023x^{4} + 0.0018x^{3} + 0.0003x^{2}$$

2-2′-3-3′-5-5′-6-6′- OCTACHLORO BIPHENYL

$$x^{20} - 7.1472x^{18} - 7.1224x^{17} + 11.5784x^{16} + 24.2113x^{15} + 8.1415x^{14} - 13.9592x^{13}$$
$$-14.7691x^{12} - 2.5071x^{11} + 4.0579x^{10} + 2.8359x^{9} + 0.4616x^{8} - 0.2725x^{7}$$
$$-0.1653x^{6} - 0.0341x^{5} - 0.0004x^{4} + 0.0012x^{3} + 0.0003x^{2}$$

APPENDIX III

CHARACTERISTIC ROOTS OF PCB CONGENERS

BIPHENYL
x_1 = 0.1315
x_2 = -0.2320
x_3 = -0.3046
x_4 = -0.4941
x_5 = -0.4941
x_6 = -0.5788
x_7 = 0.7826
x_8 = 1.4942
$x_{10} = x_{11} = x_{12} = 0.0000$

2-CHLORO BIPHENYL
x_1 = -0.3792
x_2 = -0.3792
x_3 = -0.6605
x_4 = -0.5684
x_5 = -0.5684
x_6 = 0.2408
x_7 = 0.0925
x_8 = -0.1683
x_9 = -0.1683
x_{10} = 0.8760
x_{11} = 1.6834
$x_{12} = x_{13} = 0.0000$

4-CHLORO BIPHENYL
x_1 = -0.6446
x_2 = -0.5562
x_3 = -0.5562
x_4 = -0.3995
x_5 = -0.3995
x_6 = 0.9509
x_7 = 0.2216
x_8 = -0.1982
x_9 = -0.1982
x_{10} = 0.9720
x_{11} = 1.6641
$x_{12} = x_{13} = 0.0000$

2-2'- DICHLORO BIPHENYL
x_1 = -0.2388
x_2 = -0.2388
x_3 = -0.6423
x_4 = -0.6423
x_5 = -0.4584
x_6 = -0.4584
x_7 = -0.7266
x_8 = 0.2552
x_9 = 0.2552
x_{10} = 1.0274
x_{11} = 1.8678
$x_{12} = x_{13} = x_{14} = 0.0000$

4-4'- DICHLORO BIPHENYL
x_1 = -0.4645
x_2 = -0.4645
x_3 = -0.1255
x_4 = -0.1255
x_5 = -0.7309
x_6 = -0.7309
x_7 = 0.2697
x_8 = 0.2697
x_9 = -0.8319
x_{10} = 1.1789
x_{11} = 1.7556
$x_{12} = x_{13} = x_{14} = 0.0000$

2-5- DICHLORO BIPHENYL
x_1 = -0.1102
x_2 = -0.4512
x_3 = -0.4512
x_4 = 0.1252
x_5 = 0.5045
x_6 = -0.6263
x_7 = -0.6263
x_8 = -0.2428
x_9 = -0.4228
x_{10} = -0.7042
x_{11} = 0.9526
x_{12} = 1.8729
$x_{13} = x_{14} = 0.0000$

2-6- DICHLORO BIPHENYL

x_1 = -0.1169
x_2 = -0.4558
x_3 = -0.4558
x_4 = -0.6095
x_5 = -0.6095
x_6 = -0.2679
x_7 = -0.2679
x_8 = -0.6533
x_9 = 0.4556
x_{10} = 0.1631
x_{11} = 0.9123
x_{12} = 1.9059
x_{13} = x_{14} = 0.0000

2-4′ DICHLORO BIPHEYNL

x_1 = -0.1317
x_2 = -0.5815
x_3 = -0.5815
x_4 = -0.4326
x_5 = -0.4326
x_6 = -0.2829
x_7 = -0.2829
x_8 = 0.2478
x_9 = 0.2478
x_{10} = -0.7061
x_{11} = 1.1177
x_{12} = 1.8187
x_{13} = x_{14} = 0.0000

3-4- DICHLORO BIPHENYL

x_1 = -0.1718
x_2 = -0.3761
x_3 = -0.6356
x_4 = -0.6356
x_5 = -0.5132
x_6 = -0.5132
x_7 = -0.2874
x_8 = -0.2874
x_9 = 0.2500
x_{10} = 0.2229
x_{11} = 1.0449
x_{12} = 1.9098
x_{13} = x_{14} = 0.0000

3-3′- DICHLORO BIPHENIYL

x_1 = -0.1065
x_2 = -0.4268
x_3 = -0.5043
x_4 = -0.5043
x_5 = -0.6718
x_6 = -0.6718
x_7 = -0.2807
x_8 = -0.2807
x_9 = 0.2909
x_{10} = 0.2153
x_{11} = 1.1387
x_{12} = 1.8021
x_{13} = x_{14} = 0.0000

2-2′-4- TRICHLORO

x_1 = 0.0737
x_2 = -0.6810
x_3 = -0.6810
x_4 = -0.4443
x_5 = -0.4443
x_6 = -0.2410
x_7 = -0.2410
x_8 = -0.6005
x_9 = -0.6005
x_{10} = 0.3895
x_{11} = 0.2925
x_{12} = 1.1849
x_{13} = 1.9932
x_{14} = x_{15} = 0.0000

2-2′-3- TRICHLORO

x_1 = 0.1659
x_2 = -0.6216
x_3 = -0.6216
x_4 = -0.4282
x_5 = -0.4282
x_6 = 0.2865
x_7 = 0.2865
x_8 = -0.1994
x_9 = -0.1994
x_{10} = -0.7240
x_{11} = -0.7240
x_{12} = 1.1788
x_{13} = 2.0289
x_{14} = x_{15} = 0.0000

2-3-4'- TRICHLORO

$x_1 = -0.0568$
$x_2 = -0.0568$
$x_3 = 0.6378$
$x_4 = 0.1170$
$x_5 = -0.7213$
$x_6 = -0.7213$
$x_7 = -0.0437$
$x_8 = -0.0437$
$x_9 = -1.1601$
$x_{10} = -1.1601$
$x_{11} = 1.2195$
$x_{12} = 1.9894$
$x_{13} = x_{14} = x_{15} = 0.0000$

2-3-3- TRICHLORO

$x_1 = 0.0843$
$x_2 = -0.6916$
$x_3 = -0.6916$
$x_4 = -0.4359$
$x_5 = -0.4359$
$x_6 = -0.6098$
$x_7 = -0.6098$
$x_8 = -0.2246$
$x_9 = -0.2246$
$x_{10} = 0.3062$
$x_{11} = 1.3062$
$x_{12} = 1.2284$
$x_{13} = 1.9099$
$x_{14} = x_{15} = 0.0000$

2-4-4'- TRICHLORO

$x_1 = -0.5905$
$x_2 = -0.5905$
$x_3 = -0.4361$
$x_4 = -0.4361$
$x_5 = -0.2440$
$x_6 = -0.2440$
$x_7 = -0.6742$
$x_8 = -0.6742$
$x_9 = 0.4354$
$x_{10} = 0.2524$
$x_{11} = 1.2435$
$x_{12} = 1.9586$
$x_{13} = x_{14} = x_{15} = 0.0000$

2-4'-5- TRICHLORO

$x_1 = -0.5056$
$x_2 = -0.5056$
$x_3 = -0.2865$
$x_4 = -0.2865$
$x_5 = -0.1147$
$x_6 = -0.1147$
$x_7 = 0.5184$
$x_8 = 0.2464$
$x_9 = -0.6812$
$x_{10} = -0.6812$
$x_{11} = -0.7545$
$x_{12} = 1.2183$
$x_{13} = 1.9478$
$x_{14} = x_{15} = 0.0000$

3-4-4'- TRICHLORO

$x_1 = -0.6970$
$x_2 = -0.6970$
$x_3 = -0.4247$
$x_4 = -0.4247$
$x_5 = -0.2095$
$x_6 = -0.2095$
$x_7 = -0.6115$
$x_8 = -0.6115$
$x_9 = 0.3701$
$x_{10} = 1.2585$
$x_{11} = 1.3068$
$x_{12} = 1.9501$
$x_{13} = x_{14} = x_{15} = 0.0000$

2-4-5- TRICHLORO

$x_1 = -0.5687$
$x_2 = -0.0016$
$x_3 = -0.0803$
$x_4 = -0.3079$
$x_5 = -0.3079$
$x_6 = -0.6871$
$x_7 = -0.6871$
$x_8 = -0.5233$
$x_9 = -0.5233$
$x_{10} = 0.5370$
$x_{11} = 0.2608$
$x_{12} = 1.0533$
$x_{13} = 2.0788$
$x_{14} = x_{15} = 0.0000$

2-2′-5- TRICHLORO

x_1 = 0.0537
x_2 = -0.6133
x_3 = -0.6133
x_4 = -0.4127
x_5 = -0.4127
x_6 = -0.2003
x_7 = -0.2003
x_8 = -0.7496
x_9 = -0.7496
x_{10} = 0.5062
x_{11} = 0.2626
x_{12} = 1.1349
x_{13} = 1.9946
$x_{14} = x_{15} = 0.0000$

2-4-6- TRICHLORO

x_1 = -0.7459
x_2 = -0.7459
x_3 = -0.4125
x_4 = -0.4125
x_5 = -0.1961
x_6 = -0.1961
x_7 = -0.6166
x_8 = -0.6166
x_9 = 0.4685
x_{10} = 0.3745
x_{11} = 1.0163
x_{12} = 2.0831
$x_{13} = x_{14} = x_{15} = 0.0000$

2-2′-3-4- TETRACHLORO

x_1 = -0.3709
x_2 = -0.3709
x_3 = 0.1970
x_4 = -0.7643
x_5 = -0.7184
x_6 = -0.7184
x_7 = -0.5690
x_8 = -0.5690
x_9 = -0.1709
x_{10} = -0.1709
x_{11} = 0.4405
x_{12} = 0.3113
x_{13} = 1.2819
x_{14} = 2.1922
$x_{15} = x_{16} = 0.0000$

2-2′-4-5′- TETRACHLORO

x_1 = 0.2107
x_2 = 0.5451
x_3 = 0.2816
x_4 = -0.3685
x_5 = -0.3685
x_6 = -0.1547
x_7 = -0.1547
x_8 = -0.7897
x_9 = -0.7331
x_{10} = -0.7331
x_{11} = -0.5793
x_{12} = -0.5793
x_{13} = 1.2644
x_{14} = 2.1592
$x_{15} = x_{16} = 0.0000$

2-2′-3-5′ TETRACHLORO

x_1 = -0.1614
x_2 = -0.1614
x_3 = 0.2103
x_4 = 0.5158
x_5 = 0.2983
x_6 = -0.7752
x_7 = -0.7207
x_8 = -0.7207
x_9 = -0.5830
x_{10} = -0.5830
x_{11} = -0.3790
x_{12} = -0.3790
x_{13} = 1.3176
x_{14} = 2.1214
$x_{15} = x_{16} = 0.0000$

2-2′-4-4′-TETRACHLORO

x_1 = -0.0899
x_2 = -0.7082
x_3 = -0.7082
x_4 = -0.4827
x_5 = -0.4827
x_6 = -0.6669
x_7 = -0.6669
x_8 = -0.2562
x_9 = -0.2562
x_{10} = 0.4765
x_{11} = 0.3492
x_{12} = 1.3382
x_{13} = 2.1545
$x_{14} = x_{15} = x_{16} = 0.0000$

2-2′-5-5′- TETRACHLORO

x_1 = 0.1119
x_2 = -0.1600
x_3 = -0.1600
x_4 = -0.3776
x_5 = -0.3776
x_6 = -0.7819
x_7 = -0.7313
x_8 = -0.7313
x_9 = -0.5869
x_{10} = -0.5869
x_{11} = 0.5320
x_{12} = 0.4883
x_{13} = 1.2662
x_{14} = 2.0954
$x_{15} = x_{16}$ = 0.0000

2-3′-4-4′- TETRACHLORO

x_1 = 0.1947
x_2 = 0.4897
x_3 = 0.2935
x_4 = -0.2147
x_5 = -0.2147
x_6 = -0.3814
x_7 = -0.4441
x_8 = -0.4441
x_9 = -0.7337
x_{10} = -0.7337
x_{11} = -0.6374
x_{12} = -0.6374
x_{13} = 1.4040
x_{14} = 2.0595
$x_{15} = x_{16}$ = 0.0000

2-3′-4′-5- TETRACHLORO

x_1 = -0.2477
x_2 = -0.1732
x_3 = -0.1732
x_4 = -0.7272
x_5 = -0.7272
x_6 = -0.5667
x_7 = -0.5667
x_8 = -0.3722
x_9 = -0.3722
x_{10} = -0.7965
x_{11} = 0.3988
x_{12} = 0.3988
x_{13} = 1.1930
x_{14} = 2.2370
$x_{15} = x_{16}$ = 0.0000

2-2′-3-3′ TETRACHLORO

x_1 = 0.3568
x_2 = -0.6979
x_3 = -0.7241
x_4 = -0.7241
x_5 = -0.5858
x_6 = -0.5858
x_7 = -0.3829
x_8 = -0.3829
x_9 = -0.1656
x_{10} = -0.1656
x_{11} = 0.2721
x_{12} = 0.2721
x_{13} = 1.3697
x_{14} = 2.1440
$x_{15} = x_{16}$ = 0.0000

2-2′-6-6′- TETRACHLORO

x_1 = 0.1641
x_2 = -0.3862
x_3 = -0.3862
x_4 = -0.7426
x_5 = -0.7011
x_6 = -0.7011
x_7 = -0.5612
x_8 = -0.5612
x_9 = -0.1895
x_{10} = -0.1895
x_{11} = 0.4525
x_{12} = 0.4406
x_{13} = 1.1388
x_{14} = 2.2230
$x_{15} = x_{16}$ =0.0000

3-3′-4-4′- TETRACHLORO

x_1 = 0.3935
x_2 = 0.2898
x_3 = 0.2014
x_4 = -0.1725
x_5 = -0.1725
x_6 = -0.4447
x_7 = -0.4447
x_8 = -0.3858
x_9 = -0.3858
x_{10} = -0.7620
x_{11} = -0.7620
x_{12} = -0.9041
x_{13} = 1.4849
x_{14} = 2.0647
$x_{15} = x_{16}$ = 0.0000

2-3-5-6- TETRACHLORO

x_1 = -0.2964
x_2 = -0.2964
x_3 = -0.1785
x_4 = -0.1785
x_5 = -0.2264
x_6 = -0.2264
x_7 = 1.6193
x_8 = 1.6193
x_9 = 0.3647
x_{10} = 0.5834
x_{11} = -2.4436
x_{12} = -0.1703
x_{13} = -0.1703
$x_{14} = x_{15} = x_{16} = 0.0000$

2-4-4'-5- TETRACHLORO

x_1 = 0.0728
x_2 = -0.3644
x_3 = -0.3644
x_4 = -0.5706
x_5 = -0.5706
x_6 = -0.7242
x_7 = -0.7242
x_8 = -0.1644
x_9 = -0.1644
x_{10} = -0.7698
x_{11} = 0.5718
x_{12} = 0.3296
x_{13} = 1.3235
x_{14} = 2.1194
$x_{15} = x_{16} = 0.0000$

2-3-4-5- TETRACHLORO

x_1 = -0.5600
x_2 = -0.5600
x_3 = -0.3610
x_4 = -0.3610
x_5 = -0.7629
x_6 = -0.7071
x_7 = -0.7071
x_8 = -0.1637
x_9 = -0.1637
x_{10} = 0.6362
x_{11} = 0.3292
x_{12} = 1.0839
x_{13} = 2.2975
$x_{14} = x_{15} = x_{16} = 0.0000$

2-2'-5-6'- TETRACHLORO

x_1 = 0.5084
x_2 = 0.4587
x_3 = 0.1560
x_4 = -0.7036
x_5 = -0.7036
x_6 = -0.5901
x_7 = -0.5901
x_8 = -0.3976
x_9 = -0.3976
x_{10} = 1.2226
x_{11} = 2.1305
x_{12} = -0.1836
x_{13} = -0.1836
x_{14} = -0.7264
$x_{15} = x_{16} = 0.0000$

2-3'-4-4'-5- PENTACHLORO

x_1 = -0.3063
x_2 = -0.3063
x_3 = -0.5127
x_4 = -0.5127
x_5 = -0.6962
x_6 = -0.6962
x_7 = 0.2567
x_8 = -0.1376
x_9 = -0.1376
x_{10} = -0.8049
x_{11} = -0.8049
x_{12} = 0.5809
x_{13} = 0.3435
x_{14} = 1.5302
x_{15} = 2.2044
$x_{16} = x_{17} = 0.0000$

2-3-3'-4'-6- PENTACHLORO

x_1 = -0.8054
x_2 = -0.7468
x_3 = -0.7468
x_4 = -0.4227
x_5 = -0.4227
x_6 = -0.6187
x_7 = -0.6187
x_8 = 2.2555
x_9 = -0.0981
x_{10} = -0.2064
x_{11} = -0.2064
x_{12} = 0.5920
x_{13} = 0.3341
x_{14} = 1.4477
x_{15} = 2.2338
$x_{16} = x_{17} = 0.0000$

2-3-3′-4-4′- PENTACHLORO

$x_1 = -0.6714$
$x_2 = -0.6714$
$x_3 = -0.5368$
$x_4 = -0.5368$
$x_5 = -0.7571$
$x_6 = -0.7571$
$x_7 = 0.2866$
$x_8 = 0.5071$
$x_9 = 0.3933$
$x_{10} = -0.1456$
$x_{11} = -0.1456$
$x_{12} = -0.3378$
$x_{13} = -0.3378$
$x_{14} = 1.4814$
$x_{15} = 2.2294$
$x_{16} = x_{17} = 0.0000$

2-3-4-5-6- PENTACHLORO

$x_1 = -0.4150$
$x_2 = -0.4150$
$x_3 = -0.2052$
$x_4 = -0.2052$
$x_5 = -0.7539$
$x_6 = -0.7539$
$x_7 = -0.0284$
$x_8 = -0.0284$
$x_9 = -0.6126$
$x_{10} = -0.6126$
$x_{11} = -0.7813$
$x_{12} = 0.7537$
$x_{13} = 0.4651$
$x_{14} = 1.1242$
$x_{15} = 2.4734$
$x_{16} = x_{17} = 0.0000$

2-2′-3-4-4′- PENTACHLORO

$x_1 = -0.1366$
$x_2 = -0.1366$
$x_3 = -0.5312$
$x_4 = -0.5312$
$x_5 = -0.6840$
$x_6 = -0.6840$
$x_7 = 0.2771$
$x_8 = -0.3292$
$x_9 = -0.3292$
$x_{10} = -0.7713$
$x_{11} = -0.7713$
$x_{12} = 0.5031$
$x_{13} = 0.3894$
$x_{14} = 1.4872$
$x_{15} = 2.2479$
$x_{16} = x_{17} = 0.0000$

2-2′-3-5′-6- PENTACHLORO

$x_1 = -0.7769$
$x_2 = -0.7285$
$x_3 = -0.7285$
$x_4 = -0.3792$
$x_5 = -0.3792$
$x_6 = 0.2485$
$x_7 = -0.4548$
$x_8 = -0.5845$
$x_9 = -0.5845$
$x_{10} = -0.1698$
$x_{11} = -0.1698$
$x_{12} = 0.5857$
$x_{13} = 0.5084$
$x_{14} = 1.3510$
$x_{15} = 2.2623$
$x_{16} = x_{17} = 0.0000$

2-2′-4-6-6′- PENTACHLORO

$x_1 = -0.8006$
$x_2 = -0.7302$
$x_3 = -0.7302$
$x_4 = -0.2455$
$x_5 = -0.2455$
$x_6 = -0.5746$
$x_7 = -0.5746$
$x_8 = 0.4160$
$x_9 = 0.4160$
$x_{10} = -0.4402$
$x_{11} = -0.4402$
$x_{12} = -0.4840$
$x_{13} = 0.1539$
$x_{14} = 1.3432$
$x_{15} = 2.2768$
$x_{16} = x_{17} = 0.0000$

2-2′-3-4′-5′- PENTACHLORO

$x_1 = -0.5386$
$x_2 = -0.5386$
$x_3 = -0.1333$
$x_4 = -0.1333$
$x_5 = -0.3373$
$x_6 = 0.3373$
$x_7 = 0.5312$
$x_8 = 0.4386$
$x_9 = 0.2702$
$x_{10} = -0.7745$
$x_{11} = -0.7745$
$x_{12} = -0.6856$
$x_{13} = -0.6856$
$x_{14} = 1.4434$
$x_{15} = 2.2554$
$x_{16} = x_{17} = 0.0000$

2-2′-3′-4-5- PENTACHLORO

x_1 = 0.5657
x_2 = 0.3302
x_3 = 0.2752
x_4 = -0.1037
x_5 = -0.4326
x_6 = -0.4326
x_7 = -0.2196
x_8 = -0.2196
x_9 = -0.6068
x_{10} = -0.6068
x_{11} = -0.7366
x_{12} = -0.7366
x_{13} = -0.7951
x_{14} = 1.4749
x_{15} = 2.2443
$x_{16} = x_{17}$ = 0.0000

2-2′-4-4′-5- PENTACHLORO

x_1 = 0.5786
x_2 = 0.4114
x_3 = 0.2571
x_4 = -0.2347
x_5 = -0.7406
x_6 = -0.7406
x_7 = -0.6076
x_8 = -0.6076
x_9 = -0.4084
x_{10} = -0.4084
x_{11} = -0.1995
x_{12} = -0.1995
x_{13} = -0.7837
x_{14} = 1.4629
x_{15} = 2.2207
$x_{16} = x_{17}$ = 0.0000

2-2′-4-5-5′- PENTACHLORO

x_1 = 0.5734
x_2 = 0.4953
x_3 = 0.2549
x_4 = -0.5302
x_5 = -0.5302
x_6 = -0.1313
x_7 = -0.1313
x_8 = -0.6879
x_9 = -0.6879
x_{10} = -0.3376
x_{11} = -0.3376
x_{12} = -0.7987
x_{13} = -0.7987
x_{14} = 1.4193
x_{15} = 2.2286
$x_{16} = x_{17}$ = 0.0000

2-2′-4-4′-6-6′-HEXACHLORO

x_1 = -0.4939
x_2 = -0.4939
x_3 = -0.2986
x_4 = -0.2986
x_5 = 0.4952
x_6 = 0.4952
x_7 = 0.4467
x_8 = 0.2328
x_9 = -0.7885
x_{10} = -0.7885
x_{11} = -0.8298
x_{12} = -0.6672
x_{13} = -0.6672
x_{14} = -0.1041
x_{15} = -0.1041
x_{16} = 1.5039
x_{17} = 2.3607
x_{18} = 0.0000

2-2′-3-3′-6-6′- HEXACHLORO

x_1 = 0.6087
x_2 = 0.5557
x_3 = 0.3183
x_4 = 0.0552
x_5 = -0.1693
x_6 = -0.1693
x_7 = -0.3770
x_8 = -0.3770
x_9 = -0.5799
x_{10} = -0.5799
x_{11} = -0.8321
x_{12} = -0.8321
x_{13} = -0.7413
x_{14} = -0.7413
x_{15} = 1.4656
x_{16} = 2.3959
$x_{17} = x_{18}$ = 0.0000

2-2′-3-4-4′-5- HEXACHLORO

x_1 = -0.0883
x_2 = -0.0883
x_3 = -0.4575
x_4 = -0.4575
x_5 = -0.2487
x_6 = -0.2487
x_7 = -0.6504
x_8 = -0.6504
x_9 = 0.3053
x_{10} = 0.6075
x_{11} = 0.5088
x_{12} = -0.8468
x_{13} = -0.7915
x_{14} = -0.7915
x_{15} = 1.5160
x_{16} = 2.3822
$x_{17} = x_{18}$ = 0.0000

2-2′-3-4-5-5′- HEXACHLORO

x_1 = -0.8082
x_2 = -0.8082
x_3 = -0.5586
x_4 = -0.5586
x_5 = -0.7195
x_6 = -0.7195
x_7 = -0.1412
x_8 = -0.1412
x_9 = 0.3307
x_{10} = -0.2448
x_{11} = -0.3586
x_{12} = -0.3506
x_{13} = 0.6442
x_{14} = 0.5272
x_{15} = 1.4962
x_{16} = 2.4030
$x_{17} = x_{18} = 0.0000$

2-2′-3-4′-5-5′- HEXACHLORO

x_1 = -0.8083
x_2 = -0.8083
x_3 = -0.4097
x_4 = -0.4097
x_5 = -0.6887
x_6 = -0.6887
x_7 = -0.3355
x_8 = 0.5866
x_9 = 0.5592
x_{10} = -0.0989
x_{11} = -0.2298
x_{12} = -0.2298
x_{13} = -0.5089
x_{14} = -0.5089
x_{15} = 1.5706
x_{16} = 2.3380
$x_{17} = x_{18} = 0.0000$

2-2′-4-6′-5-5′- HEXACHLORO

x_1 = -0.5800
x_2 = -0.5800
x_3 = -0.1687
x_4 = -0.1687
x_5 = -0.7305
x_6 = -0.7305
x_7 = -0.3811
x_8 = -0.3811
x_9 = -0.8279
x_{10} = -0.8279
x_{11} = 0.3237
x_{12} = 0.6224
x_{13} = 0.5119
x_{14} = 1.5967
x_{15} = 2.3220
$x_{16} = x_{17} = x_{18} = 0.0000$

2-2′-4-5-5′-6- HEXACHLORO

x_1 = -0.0396
x_2 = -0.0396
x_3 = 0.2214
x_4 = -0.1165
x_5 = -0.5018
x_6 = -0.5018
x_7 = 0.0041
x_8 = 0.0041
x_9 = -1.1906
x_{10} = -1.1906
x_{11} = -0.9384
x_{12} = -0.9384
x_{13} = 0.6803
x_{14} = 0.6803
x_{15} = 1.4628
x_{16} = 2.4041
$x_{17} = x_{18} = 0.0000$

2-2′-3-3′-4-4′- HEXACHLORO

x_1 = 0.5252
x_2 = 0.4264
x_3 = 0.3417
x_4 = -0.1708
x_5 = -0.1708
x_6 = -0.7253
x_7 = -0.7253
x_8 = -0.8349
x_9 = -0.8349
x_{10} = -0.5567
x_{11} = -0.5567
x_{12} = -0.3683
x_{13} = -0.3683
x_{14} = 1.6568
x_{15} = 2.3622
$x_{16} = x_{17} = x_{18} = 0.0000$

2-2′-4-4′-5-5′- HEXACHLORO

x_1 = 0.2499
x_2 = 0.6280
x_3 = 0.5101
x_4 = -0.3258
x_5 = -0.1241
x_6 = -0.6811
x_7 = -0.7905
x_8 = -0.7905
x_9 = -0.6621
x_{10} = -0.6621
x_{11} = -0.4695
x_{12} = -0.4695
x_{13} = -0.2476
x_{14} = -0.2476
x_{15} = 1.6049
x_{16} = 2.3262
$x_{17} = x_{18} = 0.0000$

2-2′-3-3′-4-4′-6-HEPTACHLORO

x_1 = -0.5282
x_2 = 0.1019
x_3 = -0.5755
x_4 = -0.5755
x_5 = -0.7303
x_6 = -0.7303
x_7 = -0.1731
x_8 = -0.1731
x_9 = 0.4102
x_{10} = -0.8003
x_{11} = -0.8003
x_{12} = -0.3801
x_{13} = -0.3801
x_{14} = 0.6252
x_{15} = 0.5260
x_{16} = 1.7007
x_{17} = 2.4829
$x_{18} = x_{19} = 0.0000$

2-2′-3-3′-5-5′-6-6′- OCTACHLORO

x_1 = -0.6686
x_2 = -0.6686
x_3 = -0.2757
x_4 = -0.2757
x_5 = -0.0877
x_6 = -0.0877
x_7 = -0.8723
x_8 = -0.8723
x_9 = -0.8022
x_{10} = -0.8022
x_{11} = -0.4850
x_{12} = -0.4850
x_{13} = 0.7168
x_{14} = 0.7214
x_{15} = 0.4630
x_{16} = 0.1965
x_{17} = 1.6784
x_{18} = 2.6070
$x_{19} = x_{20} = 0.0000$

2-2′-3-3′-4-4′-5-5′-OCTACHLORO

x_1 = -0.7377
x_2 = -0.8550
x_3 = -0.8062
x_4 = -0.8062
x_5 = -0.0927
x_6 = -0.0927
x_7 = -0.4931
x_8 = -0.4931
x_9 = -0.6800
x_{10} = -0.6800
x_{11} = 0.4792
x_{12} = 0.6553
x_{13} = 0.6553
x_{14} = 0.1004
x_{15} = -0.2833
x_{16} = -0.2833
x_{17} = 1.8304
x_{18} = 2.5829
$x_{19} = x_{20} = 0.0000$

2-2′-3-3′-4-5′-6-6′-OCTACHLORO

x_1 = -0.7381
x_2 = -0.7381
x_3 = -0.6700
x_4 = -0.6700
x_5 = -0.3231
x_6 = -0.3231
x_7 = -0.1106
x_8 = -0.1106
x_9 = -0.8202
x_{10} = -0.8202
x_{11} = -0.5314
x_{12} = -0.5314
x_{13} = 0.4921
x_{14} = 0.7192
x_{15} = 0.6192
x_{16} = 0.2383
x_{17} = 1.7057
x_{18} = 2.6124
$x_{19} = x_{20} = 0.0000$

APPENDIX IV

```
PROGRAM BUILDMAT;
(* CREATE MATRIX FILE FROM DATA ENTERED AT TERMINAL *)

TYPE
    MATRIX=RECORD
      ORIMAT:ARRAY[1..40] OF REAL;
    END;
    MATFILE=FILE OF MATRIX;
    REALARRAY=ARRAY[1..40,1..40] OF REAL;

VAR
   OUTFILE:MATFILE;
   REC:MATRIX;
   MORE:CHAR;
   ORMAT:REALARRAY;
   NAME:STRING[8];
   N,H,V,K:INTEGER;

BEGIN
     (* READ FILE NAME *)
     WRITE('FILE NAME :'); READ(NAME);
     (* OPEN FILE INVENTORY *)
     ASSIGN(OUTFILE,NAME);
     RESET(OUTFILE);

     (* READ ALL MATRIX DATA AND UPDATE MATRIX FILE *)
     READ(OUTFILE,REC);
     N:=0;
     FOR V:=1 TO 40 DO
       BEGIN
         IF REC.ORIMAT[V]<998 THEN N:=N+1;
       END;
     FOR H:=1 TO N DO
       BEGIN
         FOR V:=1 TO 40 DO
           BEGIN
             ORMAT[H,V]:=REC.ORIMAT[V];
           END;
         IF H<N THEN READ(OUTFILE,REC);
       END;
     (* SHOW THE ROW OF THE MATRIX *);
     WRITE ('WHICH ROW DO YOU WANT TO UPDATE');
     READLN(K);
     WHILE K<>0 DO
       BEGIN
         FOR V:=1 TO N DO
           WRITE(ORMAT[K,V]:8:4);
         WRITELN;
         WRITE('WHICH ELEMENT DO YOU WANT TO UPDATE');
         WRITE('GIVE 0 AS SENTINEL');
         READLN(V);
         WHILE V<>0 DO
           BEGIN
             WRITE(K,'.',V,':');
             READLN(ORMAT[K,V]);
             WRITE('WHICH ELEMENT DO YOU WANT TO UPDATE');
             WRITE('GIVE 0 AS SENTINEL');
             READLN(V);
           END;
         WRITE('WHICH ROW DO YOU WANT TO UPDATE');
```

```
      READLN(K);
    END;
  FOR H:=1 TO N DO
    BEGIN
      FOR V:=1 TO N DO
        BEGIN
          REC.ORIMAT[V]:=ORMAT[H,V];
        END;
      FOR V:=N+1 TO 40 DO
        BEGIN
          REC.ORIMAT[V]:=999;
        END;
      SEEK(OUTFILE,H-1);
      WRITE(OUTFILE,REC);
    END;
  (* CLOSE OUTFILE FILE *);
  WRITELN('FILE',NAME,'UPDATED');
  CLOSE(OUTFILE)
ND.
```

```
PROGRAM BUILDMAT;
(* CREATE MATRIX FILE FROM DATA ENTERED AT TERMINAL *)

TYPE
    MATRIX=RECORD
      ORIMAT:ARRAY[1..40] OF REAL;
    END;
    MATFILE=FILE OF MATRIX;
    REALARRAY=ARRAY[1..40,1..40] OF REAL;

VAR
   OUTFILE:MATFILE;
   REC:MATRIX;
   MORE:CHAR;
   ORMAT:REALARRAY;
   NAME:STRING[8];
   N,H,V,K:INTEGER;

BEGIN
     (* READ FILE NAME *)
     WRITE('FILE NAME :'); READ(NAME);
     (* OPEN FILE INVENTORY *)
     ASSIGN(OUTFILE,NAME);
     REWRITE(OUTFILE);

     (* READ ALL MATRIX DATA AND CREATE MATRIX FILE *)
     WRITE ('GIVE THE DIMENSION OF THE MATRIX');
     READLN(N);
     FOR H:=1 TO N DO
       BEGIN
         WRITELN;
         FOR V:=1 TO N DO
           BEGIN
             WRITE(H,'.',V,':');
             READ(ORMAT[H,V]);
             WRITE(' ');
           END;
       END;
     (* SHOW THE ROW OF THE MATRIX *);
     WRITE ('WHICH ROW DO YOU WANT TO UPDATE');
     READLN(K);
     WHILE K<>0 DO
       BEGIN
         FOR V:=1 TO N DO
           WRITE(ORMAT[K,V]:8:4);
         WRITELN;
         WRITE('WHICH ELEMENT DO YOU WANT TO UPDATE');
         WRITE('GIVE 0 AS SENTINEL');
         READLN(V);
         WHILE V<>0 DO
           BEGIN
             WRITE(K,'.',V,':');
             READLN(ORMAT[K,V]);
             WRITE('WHICH ELEMENT DO YOU WANT TO UPDATE');
             WRITE('GIVE 0 AS SENTINEL');
             READLN(V);
           END;
         WRITE('WHICH ROW DO YOU WANT TO UPDATE');
         READLN(K);
       END;
```

```
    FOR H:=1 TO N DO
      BEGIN
        FOR V:=1 TO N DO
          BEGIN
            REC.ORIMAT[V]:=ORMAT[H,V];
          END;
        FOR V:=N+1 TO 40 DO
          BEGIN
            REC.ORIMAT[V]:=999;
          END;
        WRITE(OUTFILE,REC);
      END;
    (* CLOSE OUTFILE FILE *);
    WRITELN('FILE',NAME,'CREATED');
    CLOSE(OUTFILE)
END.
```

```
    PROGRAM PROJECT(INPUT,OUTPUT);
TYPE
    MATRIX=RECORD
      ORIMAT:ARRAY[1..40] OF REAL;
    END;
    MATFILE=FILE OF MATRIX;
    REALARRAY=ARRAY[1..40,1..40] OF REAL;
    AARRAY=ARRAY[0..40] OF REAL;
VAR
   OUTFILE:MATFILE;
   REC:MATRIX;
   ORMAT,B,Z:REALARRAY;
   T,A:AARRAY;
   U,I,N,H,V,MU,OKU,C1,C2,ANY,COUNT:INTEGER;
   TEMP:REAL;
   NAME:STRING[8];

BEGIN
   REPEAT
     FOR V:=1 TO 24 DO
       WRITELN(' ');
     (* READ FILE NAME *)
     WRITE('FILE NAME : '); READ(NAME);
     (* OPEN FILE OUTFILE *)
     ASSIGN(OUTFILE,NAME);
     RESET(OUTFILE);

     (* READ ALL MATRIX DATA AND FILL THE ARRAY *)
     READ(OUTFILE,REC);
     N:=0;
     FOR V:=1 TO 40 DO
       BEGIN
         IF REC.ORIMAT[V]<998 THEN N:=N+1;
       END;
     FOR H:=1 TO N DO
       BEGIN
         FOR V:=1 TO N DO
           BEGIN
             ORMAT[H,V] := REC.ORIMAT[V];
           END;
         IF H<N THEN READ(OUTFILE,REC);
       END;

     WRITELN(' ');
     WRITE('   :   ');
       FOR V:=1 TO N DO
         WRITE(V:2,'     ');
     WRITELN;
     WRITE('...');
       FOR V:=1 TO 7*N DO
         WRITE('.');
     WRITELN;
       FOR H:=1 TO N DO
         BEGIN
           WRITE(H:2,' :');
           FOR V:=1 TO N DO
             WRITE(ORMAT[H,V]:6:4,' ');
           WRITELN;
         END;
       TEMP:=0;
```

```
    FOR H:=1 TO N DO
      TEMP:=TEMP+ORMAT[H,H];
  T[0]:=1;
  A[0]:=T[0];
  T[1]:=TEMP;
  A[1]:=-T[1];
  FOR H:=1 TO N DO
    FOR V:=1 TO N DO
      Z[H,V]:=ORMAT[H,V];
  FOR I:=2 TO N DO
    BEGIN
      FOR H:=1 TO N DO
        BEGIN
          FOR V:=1 TO N DO
            BEGIN
              TEMP:=0;
              FOR ANY:=1 TO N DO
                TEMP:=TEMP+ORMAT[H,ANY]*Z[ANY,V];
                B[H,V]:=TEMP;
            END
        END;
      TEMP:=0;
        FOR H:=1 TO N DO
          TEMP:=TEMP+B[H,H];
      T[I]:=TEMP;
      TEMP:=0;
        FOR COUNT:=1 TO I DO
          TEMP:=TEMP+(-(1/I))*A[I-COUNT]*T[COUNT];
      A[I]:=TEMP;
        FOR H:=1 TO N DO
          FOR V:=1 TO N DO
            Z[H,V]:=B[H,V]
    END;
  WRITELN('                X^',N:2,' +');
  FOR I:=1 TO N DO
    BEGIN
      WRITE('(',A[I]:11:4,') ');
      IF N-I<>0 THEN
        WRITE('X^',N-I:2,' +')
      ELSE
        WRITE('      = 0');
        WRITELN;
    END;
  WRITE('PLEASE ENTER 0 AS SENTINEL OR ANY # TO GO  ');
  READ(MU);
UNTIL MU=0;
  END.
```

```
12 REM--------------------------------
14 REM---MACKAY LEVEL 1 FUGACITY MODEL
15 REM--------------------------------
16 REM---LOAD "MACKAY",8
17 REM--------------------------------
140 DIM D(6)
180 DIM P(6)
190 DIM Z(6)
200 DIM M(6)
210 DIM E(6)
220 DIM A(6)
230 DIM C(6)
240 DIM T$(6)
250 T$(1)= "******AIR"
260 T$(2)= "*****SOIL"
270 T$(3)= "****WATER"
280 T$(4)= "****BIOTA"
290 T$(5)= "S. SOLIDS"
300 T$(6)= "*SEDIMENT"
310 REM----PARAMETERS---------------
320 V(1)=6E+09
330 V(2)=45000!
340 V(3)=7000000!
350 V(4)=7
360 V(5)=35
370 V(6)=21000
380 D(1)=.00119
390 D(2)=1.5
400 D(3)=1
410 D(4)=1
420 D(5)=1.5
430 D(6)=1.5
440 P(2)=2
450 P(5)=4
460 P(6)=4
470 T=298
480 R=8.314
490 REM-----------VARIABLES-----------
540 INPUT "NAME OF CHEMICAL: ",C$
560 INPUT "MOLECULAR WEIGHT: ",M
580 INPUT "LOGP: ",P8
590 INPUT "LOGS: ",C8
700 INPUT "LOGKOW: ",L7
701 REM----CONVERSION-----------------
702 P5=(10^P8)/.0075
703 C5=(10^C8)*1000
704 H=P5/C5
705 LPRINT "NAME OF CHEMICAL:"C$
706 LPRINT
707 LPRINT "HENRY CONSTANT (Pa m3/mol):"H
708 LPRINT
710 REM----FUG CAP CONSTANT-----------
711 LPRINT "MOLECULAR WEIGHT:"M
712 LPRINT
713 LPRINT "LOGP:"P8
714 LPRINT
715 LPRINT "LOGS:"C8
716 LPRINT
717 LPRINT "LOGKOW:"L7
718 LPRINT
```

```
720 Z(1)=1/(R*T)
740 Z(3)=1/H
750 K8=10^(L7-1.32)
760 Z(4)=K8*D(4)/H
770 K2=10^(.594*L7+.78)
780 Z(5)=K2*D(5)*P(5)/H/100
790 K3=10^(.594*L7+.78)
800 Z(2)=K3*D(2)*P(2)/H/100
810 K9=10^(.594*L7+.78)
820 Z(6)=K9*D(6)*P(6)/H/100
821 LPRINT "Z1="Z(1)
822 LPRINT "Z2="Z(2)
823 LPRINT "Z3="Z(3)
824 LPRINT "Z4="Z(4)
825 LPRINT "Z5="Z(5)
826 LPRINT "Z6="Z(6)
830 REM---DIST VALUE------------------
840 S8=0
850 S5=0
860 FOR I=1 TO 6
870 S8=S8+Z(I)
880 S5=S5+Z(I)*V(I)
890 NEXT I
900 F=100/S5
910 FOR  I=1 TO 6
920 M(I)=Z(I)*V(I)/S5
930 E(I)=Z(I)/S8
940 A(I)=F*Z(I)*V(I)
950 C(I)=A(I)/V(I)*M/D(I)
960 NEXT I
980 REM PRINT DIST VALUES-------------
990 LPRINT
1000 LPRINT SPC(9)"MASS PART","EQ PART","AMOUNT","CONC"
1020 FOR I=1 TO 6
1025 LPRINT T$(I)  M(I) E(I) A(I) C(I)
1026 LPRINT
1040 NEXT I
1050 REM REPEAT PROCEDURE FOR NEW CHEM
1110 INPUT AB
1120 IF AB=1 THEN  490
1121 IF AB=0 THEN  1130
1130 END
```

APPENDIX V

FUGACITY CAPACITY CONSTANTS (Z_S, Z_W) CALCULATED FROM EXPERIMENTAL[a] AND PREDICTED[b] INPUT DATA

CONGENER NO	Z_S Calc[a]	Z_S Calc[b]	Z_W Calc[a]	Z_W Calc[b]
Biphenyl	0.83	0.84	2.24E-02	2.33E-02
2-chloro	1.06	2.08	1.55E-02	2.72E-02
4-	2.42	2.33	2.89E-02	2.78E-02
2-2'-dichloro	4.63	5.43	2.71E-02	3.19E-02
4-4'-	3.24	6.16	2.14E-02	3.25E-02
2-5-	9.53	5.94	4.88E-02	3.24E-02
2-6-	-	5.75	-	3.22E-02
2-4'-	3.17	5.21	1.58E-02	3.22E-02
3-4-	-	5.66	-	3.22E-02
3-3'-	-	5.90	-	3.26E-02
2-2'-4-trichloro	-	14.55	-	3.76E-02
2-2'-3-	-	14.92	-	3.78E-02
2-2'-5-	2.87	15.08	7.69E-03	3.79E-02
2-3-4'-	-	15.39	-	3.80E-02
2-4'-5-	-	14.49	-	3.76E-02
2-3-3'-	-	14.34	-	3.76E-02
3-4-4'-	-	13.32	-	3.71E-02
2-4-4'-	-	13.44	-	3.72E-02
2-4-5-	13.46	14.48	3.81E-02	3.76E-02
2-4-6-	13.82	14.82	3.60E-02	3.78E-02
2-2'-3-4-tetra	-	36.31	-	4.38E-02
2-2'-3-5'-	-	39.29	-	4.45E-02
2-2'-4-4'-	19.14	40.01	2.49E-02	4.64E-02
2-3-4-4'-	-	29.94	-	4.35E-02
2-2'-5-5'-	34.80	41.50	3.68E-02	4.48E-02
2-3'-4-4'-	-	37.62	-	4.41E-02
2-3'-4'-5-	66.19	40.14	7.29E-02	4.45E-02
2-2'-3-3'-	-	35.78	-	4.37E-02

CONTINUED

CONGENER NO	Z_S Calc[a]	Z_S Calc[b]	Z_W Calc[a]	Z_W Calc[b]
3-3'-4-4'-	96.14	37.21	1.09E-01	1.42E-02
2-3-5-6-	-	23.40	-	4.08E-02
2-4-4'-5-	-	35.96	-	4.38E-02
2-3-4-5-	-	31.50	-	4.28E-02
2-2'-5-6'-	-	40.20	-	4.46E-02
2-2'-6-6'	-	36.11	-	4.38E-02
2-2'-4-5-	-	39.09	-	4.44E-02
2-3'-4-4'-5-penta	-	91.25	-	5.11E-02
2-3-3'-4-4'-	-	88.38	-	5.09E-02
2-3-4-5-6-	-	75.87	-	4.96E-02
2-2'-3-4-4'-	-	89.76	-	5.11E-02
2-2'-3-5'-6-	-	98.53	-	5.18E-02
2-2'-4-6-6'-	-	94.82	-	5.15E-02
2-2'-3-4-5'-	40.83	95.43	1.92E-02	5.16E-02
2-2'-3'-4-5-	-	87.29	-	5.09E-02
2-2'-4-4'-5-	-	93.83	-	5.14E-02
2-2'-4-5-5'-	163.71	101.45	7.72E-02	5.21E-02
2-3-3'-4'-6-	-	87.45	-	5.08E-02
2-2'-3-4-4'-5-hexa	-	225.70	-	5.95E-02
2-2'-3-3'-6-6'-	196.29	194.75	9.77E-01	5.82E-02
2-2'-3-4-5-5'-	-	226.34	-	5.95E-02
2-2'-3-4'-5-5'-	-	221.82	-	5.94E-02
2-2'-4-4'-5-5'-	160.89	224.16	3.38E-02	5.95E-02
2-2'-4-5-5'-6-	-	247.63	-	6.05E-02
2-2'-3-3'-4-4'-	93.20	192.87	3.78E-02	5.80E-02
2-2'-4-4'-6-6'-	57.66	290.41	1.04E-02	6.20E-02
2-2'-3-3'-4-4'-6-	-	521.05	-	6.85E-02
2-2'-3-3'-4-4'-5-5'-	-	1223.93	-	7.90E-02
2-2'-3-3'-4-5'-6-6'-	-	1429.51	-	8.11E-02
2-2'-3-3'-5-5'-6-6'-	941.16	1421.72	5.19E-02	8.11E-02

FUGACITY CAPACITY CONSTANTS (Z_B, $Z_{SS\&ZS}$) CALCULATED FROM EXPERIMENTAL[a] AND PREDICTED[b] INPUT DATA

CONGENER NO	Z_B Calc[a]	Z_B Calc[b]	$Z_{SS\&ZS}$ Calc[a]	$Z_{SS\&ZS}$ Calc[b]
Biphenyl	8.26	8.30	1.65	1.68
2-chloro	16.25	34.36	2.12	4.16
4-	42.76	41.12	4.85	4.67
2-2'-dichloro	132.75	154.90	9.27	10.86
4-4'-	85.51	188.82	6.49	12.31
2-5-	298.57	178.67	19.06	11.89
2-6-	-	169.45	-	11.50
2-4'-	101.17	167.51	6.34	11.43
3-4-	-	165.21	-	11.32
3-3'-	-	175.81	-	11.81
2-2'-4-trichloro	-	727.88	-	29.11
2-2'-3-	-	756.94	-	29.85
2-2'-5-	138.69	769.24	5.74	30.17
2-3-4'-	-	794.43	-	30.78
2-4'-5-	-	722.87	-	28.99
2-3-3'-	-	709.67	-	28.68
3-4-4'-	-	632.50	-	26.64
2-4-4'-	-	641.30	-	26.88
2-4-5-	632.50	721.20	26.91	28.96
2-4-6-	687.17	748.27	27.64	29.65
2-2'-3-4-tetra	-	3055.35	-	72.61
2-2'-3-5'-	-	3451.92	-	78.08
2-2'-4-4'-	1531.30	3459.87	38.38	80.03
2-3-4-4'-	-	2254.55	-	59.88
2-2'-5-5'-	3206.72	3767.56	69.60	83.01
2-3'-4-4'-	-	3228.85	-	79.25
2-3'-4'-5-	5930.09	3573.23	132.38	80.29
2-2'-3-3'-	-	2985.79	-	71.86

CONTINUED

CONGENER NO	Z_B Calc[a]	Z_B Calc[b]	$Z_{SS\&Z_S}$ Calc[a]	$Z_{SS\&Z_S}$ Calc[b]
3-3′-4-4′-	8453.98	3170.02	192.28	74.43
2-3-5-6-	-	1531.30	-	46.80
2-4-4′-5-	-	3006.50	-	71.92
2-3-4-5-	-	2443.77	-	63.00
2-2′-5-6′-	-	3581.46	-	80.40
2-2′-6-6′	-	3027.34	-	72.22
2-2′-4-5-	-	3428.16	-	78.19
2-3′-4-4′-5-penta	-	12973.62	-	182.50
2-3-3′-4-4′-	-	12332.77	-	176.66
2-3-4-5-6-	-	9706.46	-	151.76
2-2′-3-4-4′-	-	12620.05	-	176.53
2-2′-3-5′-6-	-	14623.82	-	197.06
2-2′-4-6-6′-	-	13774.06	-	189.64
2-2′-3-4-5′-	6532.21	13901.48	81.68	190.85
2-2′-3′-4-5-	-	12079.84	-	174.59
2-2′-4-4′-5-	-	13553.82	-	187.65
2-2′-4-5-5′-	26185.54	15313.04	327.42	202.90
2-3-3′-4′-6-	-	12135.61	-	174.91
2-2′-3-4-4′-5-hexa	-	53710.73	-	451.40
2-2′-3-3′-6-6′-	302037.60	42565.90	3920.59	389.00
2-2′-3-4-5-5′-	-	53958.70	-	452.64
2-2′-3-4′-5-5′-	-	52247.09	-	443.64
2-2′-4-4′-5-5′-	44674.74	53095.93	321.79	448.32
2-2′-4-5-5′-6-	-	62095.58	-	495.25
2-2′-3-3′-4-4′-	16521.93	41692.81	186.40	384.37
2-2′-4-4′-6-6′-	17744.02	79810.60	115.32	580.81
2-2′-3-3′-4-4′-6-	-	199554.60	-	1042.10
2-2′-3-3′-4-4′-5-5′-	-	762184.80	-	2447.86
2-2′-3-3′-4-5′-6-6′-	-	972885.20	-	2859.85
2-2′-3-3′-5-5′-6-6′-	653224.10	963965.40	1882.51	2842.43

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