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Prediction of Gas Chromatographic Retention Times of Polychlorinated Biphenyls

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Abstract :

Two theoretical models of the relationship between the molecular structure of polychlorinated biphenyls (PCBs) and their gas chromatographic retention characteristics have been developed. The retention time of these compounds was predicted as a linear relationship between the retention times and 3D Wiener number with R of 0.990. A five-variable regression equation with R^2 of 0.997 and relative standard deviation of 1.04% was developed. Descriptors that represent 3D Wiener number, degree of chlorination and a subclass of the nonvalent and valent molecular connectivity path, cluster and /or path/ cluster type indices were among the variables included in the equation. Twenty-one commercially available PCBs are enough in order to accurately predict the retention times of all 209 PCB congeners.

Key words: Polychlorinated Biphenyls; PCB; Prediction; Gas Chromatography; Retention Time; 3D Wiener Number.

Introduction :

Polychlorinated biphenyls (PCBs) had been manufactured as commercial mixture for more than four decade before they have been banned in the U.S.A. in 1976. Because of their long-term heavy usage as dielectric fluids in transformers and capacitors, in hydraulic fluids, fire retardant etc. and their persistence, PCBs have permeated into practically every environmental medium throughout the world[1]. The persistence of the ubiquitous pollutants PCBs in the environment, offer serious difficulties to the residue analyst and toxicologist. Regulatory analysis requirements are sometimes limited to quantitation as total amount of PCB[2], as amount of specific technical mixture distributions[3] or as separate amounts of specified small subset of individual priority congeners[4,5]. There are 209 possible PCB isomers. The large number of compounds present in the commercial PCB preparation makes determination of total and individual PCB content of environmental samples with any degree of accuracy extremely difficult.

In this study, we report on two theoretical models to describe relationship between the molecular structure of polychlorinated biphenyls (PCBs) and their gas chromatographic retention characteristics. The retention time of these compounds was predicted as a linear relationship between the retention times and 3D Wiener number with R of 0.990. A five-variable regression equation with R^2 of 0.997 and relative standard deviation of 1.04% was developed. Descriptors that represent 3D Wiener number, degree of chlorination and a subclass of the nonvalent and valent molecular connectivity path, cluster and /or path/cluster type indices were among the variables included in the equation. Twenty-one commercially available PCBs are enough in order to accurately predict the retention times of all 209 PCB congeners

Method of Calculation :

Gas chromatographic retention times of PCBs were predicted following the method of quantitative structure-retention relationship (QSRR). The procedure consists of three stages: (1) entry and storage of all 209 possible PCB congeners (2) generation of molecular descriptors and (3) regression analysis. All computations were performed using software packages HyperChem 6.0, Molecular Modeling Pro and Statgraphics 3.0. The three dimensional models of structure were generated by using Molecular Mechanics calculation. Generation of molecular descriptors can be divided into four classes: (a) topological descriptors - include molecular connectivity indices and valence connectivity indices. (b) geometric descriptors - include 3D Wiener number. It is based on the distance matrix in which topographic (geometric) distances rather than topological (graph theoretical) distances are the entries (c) semi-empirical MO descriptors - include total energy, dipole moment and atomic charges (d) structure descriptors - include degree of chlorination and substitution pattern. The experimental GC retention times data used in this investigation are taken from W. Vetter, B. Luckas[16], and M. D. Mullin et al.[17]. Basically, regression equation is developed by using measured retention times as a dependent variable and molecular structure descriptors as the predictors variables.

Forty molecular descriptors were calculated for each of 209 PCBs. In single variable model, only the 3-Dimensional Wiener number (^{3D}W) is useful for predicting the experimental retention time of PCBs. Multiple linear regression performed on the forty molecular descriptors resulted in a five-descriptor equation. The descriptors used in the multiple regression are displayed in Table I. Several extensive reviews have been published and give a detailed description of the theory and method of calculating the indices used in the present investigation. In presented

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equations for the indices shown in Table I, we will use the graph-theoretical language of references[18-22].

Table I

Symbols for molecular descriptors used in regression analysis

Symbol	Type of descriptors
^{3D}W	three-dimensional Wiener number (All atoms)
Cl (sq.)	Number of Chlorine's Squared
$^{5}\chi_{PC}$	Fifth-order path/cluster connectivity index
$^{1}\chi^{v}$	First-order valence connectivity index
$^{4}\chi^{v}$	Fourth-order valence connectivity index

(i) The Wiener number may be defined for arbitrary connected graph (structure) G in the following way.

Let us assume that G has vertices 1, 2, ..., N. For each pair k, l of vertices, let $(D)_{kl}$ denote the distance in G between k and l; i.e. the length of the shortest path between k and l. The distance $(D)_{kl}$ represents the elements of the distance matrix
D = D(G) of the graph G. The Wiener number W = W(G) of G is therefore given by :

$$W = \sum_{k=1}^{N} \sum_{l=1}^{k} (D)_{kl} = \frac{1}{2} \sum_{k=1}^{N} \sum_{l=1}^{N} (D)_{kl} \quad (1)$$

In other words, the Wiener number W of G is equal to the half-sum of the elements of D. Since the distance matrix in the above formulation contains information only about the 2D structure of a molecule, we named the corresponding number representing the sum of all graph-theoretical distances in G the 2D Wiener number. We denote it by ^{2D}W.

The distance matrix of a structure may also be based on the topographic (geometric) distances, i.e. the matrix elements. $(D)_{kl}$ represents "true" spatial distances between atoms k and l in a molecule expressed in some units of length. The topographic (geometric) distance matrix contains information on the 3D structure of a molecule. The corresponding Wiener number is termed the 3D Wiener number, and it is representative of topographic invariants. We denote it by ^{3D}W (Ref. 18).

(ii) The nonvalent ($^{n}\chi_{t}$) and valent molecular connectivities ($^{n}\chi^{v}_{t}$) are calculated by considering various fragments of the molecule[19, 20] :

$$^{n}\chi_{t} = \sum_{s=1}^{n_m} \left(\prod_{i}^{m=1} \delta_i \right)_s^{-\frac{1}{2}} \quad (2)$$

$$^{n}\chi^{v}_{t} = \sum_{s=1}^{n_m} \left(\prod_{i}^{m=1} \delta^{v}_i \right)_s^{-\frac{1}{2}} \quad (3)$$

Where $^{n}\chi_{t}$ is the *n*-th order term of type *t* (*t* = path, cluster, path/cluster, or chain) n_m is the number of connected subgraphs of type *t*, *m* is the number of edges, and δ and δ^{v} are the vertex nonvalence and valence values, respectively. The nonvalence value, δ, is equal to the number of nonhydrogen atoms connected to the atom of interest and is assigned to each atom in a molecule excluding the hydrogen atoms. The valence delta value, δ^{v}, is calculated from the following equation,

$$\delta^{v} = \frac{Z^{v} - h}{Z - Z^{v} - 1} \quad (4)$$

Where Z^{v} is the number of valence electrons in the atom, *h* is the number of hydrogen atoms bound to that atom, and *Z* is its atomic number.

All topographical and topological indices were calculated according to the formulae in the references[18-20] using a computer program written in FORTRAN.

Results and Discussion :

The systematic numbering of each PCB in Table II is according to the system of K. Ballschmiter and M. Zell[9]. The N° in columns is used as a synonym for the corresponding PCB compound in tables and figures. The experimental retention times[17] and the molecular descriptors of PCBs examined in the present study are shown in Table III.

It is apparent that the retention time of substituted biphenyls is predominantly influenced by position of the chloro substituents while the influence of the number of chlorine atoms is secondary. The first compounds to be eluated are those having a chloro atom in position 2, followed by 3-substituted and finally 4-substituted derivatives[16,17]. For dichlorobiphenyls series in which one substituent is in the *ortho*-position, 2,4-dichlorobiphenyl is the one with the longest elution time. Of the *meta*- and *para*-substituted derivatives, 4,4'-dichlorobiphenyl is eluted last.

From Table III we see that the ^{3D}W is a good descriptor for predicting the linear programmed gas chromatographic retention times of PCBs. A comparative study showed that elution order of PCBs on a liquid crystal phase depends predominantly on the shape of the molecules[25, 26].

Forty molecular descriptors were tested and the best single descriptor equation for prediction of gas chromatographic Relative Retention Times (RRT) of polychlorinated biphenyls employs the 3D Wiener number (^{3D}W). The equation of the fitted model is:

$$RRT = 10.751\ (\pm 0.099) - 9973.67\ (\pm 97.136) / {}^{3D}W \qquad (5)$$

$N = 209$; $r = -0.9903$; $R^2 = 98.07\%$; $s = 0.025$; $F^{1,207} = 10542.74$; $p = 0.001$;

Since the p-value in ANOVA analysis is less than 0.01, there is a statistically significant relationship between RRT and ^{3D}W at the 99% confidence level.

Equation (5) was used to calculate the retention times of the PCBs and the values obtained are given in Table IV. Figure 1 shows a plot between experimental retention times and the predicted. Agreement between the predicted and observed retention times suggest that the gas chromatographic behavior of PCBs may depend critically on the shape of molecular network and geometry.

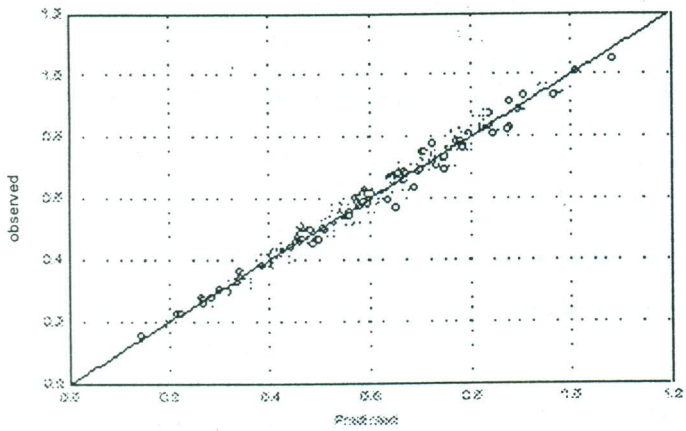

Figure 1. Plot of observed retention times versus predicted values using eq. 5

Subsequently, a multivariate model that better differentiated isomeric PCBs was developed. The stepwise variable selection procedure was used. When a high collinearity is detected ($R > 0.90$), one or more of the offending descriptors is removed from consideration. A final pool of five descriptors, as independent variables in the multiple linear regression, were obtained. The multivariate regression of retention times with five descriptors is presented in Table V, eq. 6. An examination of the residuals (Figure 2) shows a fairly random pattern. The mean absolute error (MAE) and the Durbin-Watson (DW) statistics tests the residuals to determine if there is any significant correlation based on the order in which they occur in data file. Since the MAE and DW are less than 0.01 and greater than 1.2 respectively (Table V), there is probably not any serious autocorrelation in the residuals. The correlation matrix for the five descriptors used in eq. 6 shows acceptable correlation between the parameters (Table VI). The retention times predicted by this equation are shown in Table IV and Figure 3. A plot of the experimental vs. predicted retention times yielded

$$(RRT)exp = Constant + {}^{3D}W + {}^{4}\chi^{v} + {}^{5}\chi^{pc} + Cl(sq.) + {}^{1}\chi^{v} \qquad (6)$$

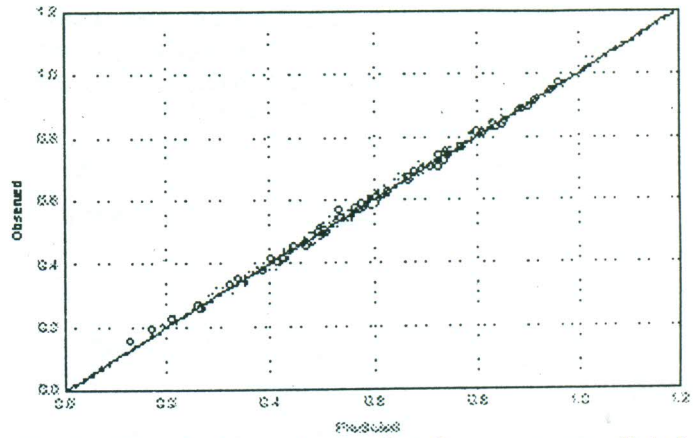

Fig. 2 : Plot of observed retention times versus predicted values using eq. 6

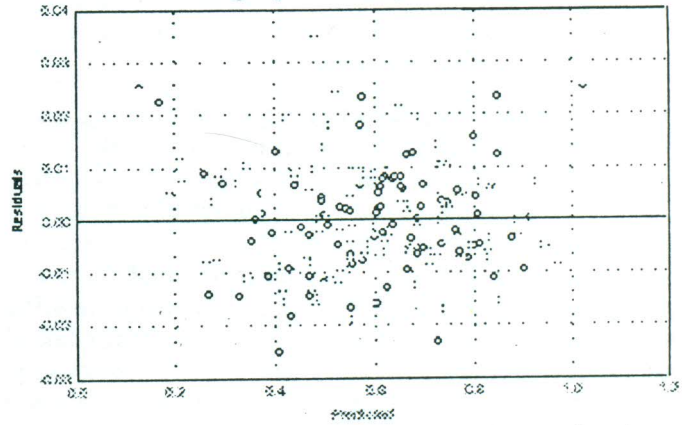

Fig. 3 : Plot of residuals versus calculated retention times using eq. 6

From all above, we get : $RRT_{exp} = a + b\ RRT_{pred}$ (7)

$N = 209$; $r = -0.9984$; $R^2 = 99.67\%$; $s = 0.010$; $F^{1,207} = 62527$; $p = 0.0001$;

As mentioned earlier, there are 209 possible PCB isomers and congeners. For many of these compounds, however, standards are not readily available in a form suitable to be used as chromatographic standards. The question is, how many commercially available PCB isomers (e.g. from Fluka Chemical Co.) are enough in order to accurately predict the retention times of all 209 congeners. The results of this study suggested that analyst can measure the retention times of 10-20 adequate by selected commercially available PCB isomers, use the retention data to build an equation, and use the equation to predict the retention of other isomers. The best single descriptor equation (with 21 isomers) for prediction of gas chromatographic RRT of PCBs employs the ^{3D}W is:

$$RRT = 10.702\ (\pm 0.175) - 9933.56\ (\pm 169.095) / {}^{3D}W \qquad (8)$$

$N = 21$; $r = -0.9973$; $R^2 = 99.45\%$; $s = 0.019$; $F^{1,19} = 3451.74$; $p = 0.001$;

Twenty-one commercially available PCBs are: 1, 2, 3, 4, 5, 7, 9, 12, 14, 15, 25, 28, 29, 52, 77, 99, 101, 137, 167, 180,

209 (see Table II, the N° in columns is used as a synonym for the corresponding PCB compound). The multivariate regression (with 21 isomers) of retention times with five descriptors is presented in Table V, eq. 9. The retention times predicted by this equation are shown in Table IV.

$$(RRT)exp_{(21)} = Constant + {}^{3D}W + {}^{4}\chi^{v} + {}^{5}\chi^{pc} + Cl(sq.) + {}^{1}\chi^{v} \quad (9)$$

A plot of the experimental vs. predicted retention times yielded :

$$RRT_{exp} = a + b\,RRT_{pred} \quad (10)$$

$N = 21$; $r = 0.9968$; $R^2 = 99.35\%$; $s = 0.014$; $F^{1,19} = 31660$; $p = 0.0001$;

When these calculations were repeated using different sets of PCB isomers, similar statistical data were obtained. We have shown that 10-20 commercially available PCBs are enough in order to accurately predict the retention times of all 209 PCB congeners.

In order to predict the gas chromatographic retention characteristics of substituted biphenyls, many authors have attempted to assign descriptors that represent their substitution pattern[11, 12, 23, 24]. Robbat et al.[12] derived position descriptors, as independent variables, to account for substitutient interaction in chlorinated biphenyls. For example, indicator TWO represents the number of chlorine atoms present at the 2,2',6 and 6' position. Position 6 and 6' are considered equivalent to position 2 and 2', respectively, Since there are four such possible position, indicator TWO can have value from 0 to 4. In the same way indicator THREE accounts for the number of chlorine atoms present at the 3,3' and 5,5' positions in the each ring and indicator FOUR those at 4 and 4'. Again, positions 5 and 5' are considered equivalent to position 3 and 3' and indicator THREE can have values from 0 to 4. Indicator FOUR can have valuês from 0 to 2 (Ref. 12).

Haas and Jus[11] predicted the gas chromatographic retention time of PCBs using descriptor variables representing the degree of chlorinating (number of chlorine atoms), number of chlorine atoms squared, number of chlorine atoms in a ortho- position, number of chlorine atoms in meta-position etc.

In the present study, a 3D Wiener number (all atoms) descriptor is used to represent the substitution pattern of PCBs. From the data in Table III, we see that ^{3D}W (as position descriptor) is the most discriminative index. For ortho-, meta- and para- chloro biphenyls ^{3D}W are 940.28, 944.86 and 946.12, respectively. In the dichlorobiphenyls series in which one substituent is in ortho- position, the largest ^{3D}W value is that of 2,4-dichlorobiphenyl and the smallest that of 2, 2'-isomer. Also it is apparent that ^{3D}W values for chlorine located at 3-, 5- or 3'-positions are not the same. 4,4'-Dichlorobiphenyl has the largest value of the dichlorobiphenyls. In the trichlorobiphenyl series the largest ^{3D}W value (970.81) is that for 3,4,4'-isomer and the smallest value (954.39) for 2,2',6-isomer. More importantly, the ^{3D}W index has a different value for each of all the possible substitution patterns of an individual ring.

On the other hand, a close inspection of the experimental data[17] (Table III) RRT values for isomeric PCB homologues are highly dependent on structure. For example, (i) for the monochlorophenyl-substituted PCB homologues RRT values increase in the order 2- < 3- < 4- with the following observed ΔRRT values: 0.04-0.05 (3-chloro- to 2-chloro-) and 0.004-0.013 (4-chloro- to 3-chloro-). (ii) For the dichlorophenyl substituted PCB homologues, the RRT values increase in the order 2,6- < 2,5- < 2,4- < 2,3- < 3,5- < 3,4-, and the observed ΔRRT values were 0.03-0.04 (2,5-dichloro- to 2,6-dichloro-), 0.004 (2,6-dichloro- to 2,5-dichloro-), 0.022 (2,3-dichloro- to 2,4-dichloro-), 0.02-0.40 (3,5-dichloro- to 2,3-dichloro-) and 0.035-0.045 (3,4-dichloro- to 3,5-dichloro). (iii) For the trichlorophenyl substituted PCB homologues, the RRT values increase in the order 2,4,6- < 2,3,6- < 2,3,5- < 2,4,5- < 2,3,4- < 3,4,5-. Experimental data from Table III reveals that 11 pairs of isomers or congeners, including 94/61, 70/76, 95/80, 60/56, 145/81, 144/135, 140/139, 133/122, 163/160, 202/171, and 203/196 exhibit similar or identical retention times. The remaining 187 PCB congeners can be separated on the fused silica capillary column coated with SE-54.

Conclusion :

We have shown that the retention time of PCBs can be predicted by using 3D Wiener number (all atoms) descriptor derived from molecular structure. ^{3D}W carries a great amount of information i.e. shape, conformation and represent the substitution pattern of PCBs. It should be noted, however, that equations were developed using retention data measured on a single stationary phase. This appears to significantly limit the usefulness of the models. However, we feel that these equations can be applied to columns of similar polarity with only slight modifications of the values of the coefficients. With availability of retention data on other stationary phase, it would be possible to assess the effects of the stationary phase polarity, column size etc.

This approach also has its limitations. At present, the three dimensional structure were generated by using Molecular Mechanics Calculation, it cannot fully account for three-dimensional problems such as for example, isomerism around the phenyl-phenyl single bond in PCBs, due to the fact that the experimental retention times were obtained with a capillary column at 270 °C and the energy supplied at this temperature is probably different than the energy barrier for rotation calculated by MM method.

3D Wiener number (all atoms) as a descriptor representing shape, conformation and the substitution pattern of PCBs, has proved to be useful and evidence suggests that it may also be applied to structurally similar compounds.

Table II

Systematic numbering of PCB compounds[9]. The number is used as a synonym for the corresponding PCB compound in tables and figures

No	Structure	No	Structure	No	Structure	No	Structure
Monochloro		53	2,2',5,6'	107	2,3,3',4',5	161	2,3,3',4,5',6
1	2	54	2,2',6,6'	108	2,3,3',4,5'	162	2,3,3',4',5,5'
2	3	55	2,3,3',4	109	2,3,3',4,6	163	2,3,3',4',5,6
3	4	56	2,3,3',4'	110	2,3,3',4',6	164	2,3,3',4',5',6
Dichloro		57	2,2',3',5	111	2,3,3',5,5'	165	2,3,3',5,5',6
4	2,2'	58	2,3,3',5'	112	2,3,3',5,6	166	2,3,4,4',5,6
5	2,3	59	2,3,3',6	113	2,3,3',5',6	167	2,3',4,4',5,5'
6	2,3'	60	2,3,4,4'	114	2,3,4,4',5	168	2,3',4,4',5',6
7	2,4	61	2,3,4,5	115	2,3,4,4',6	169	3,3',4,4',5,5'
8	2,4'	62	2,3,4,6	116	2,3,4,5,6	Heptachloro	
9	2,5	63	2,3,4',5	117	2,3,4',5,6	170	2,2',3,3',4,4',5
10	2,6	64	2,3,4',6	118	2,3',4,4',5	171	2,2',3,3',4,4',6
11	3,3'	65	2,3,5,6	119	2,3',4,4',6	172	2,2',3,3',4,5,5'
12	3,4	66	2,3',4,4'	120	2,3',4,5,5'	173	2,2',3,3',4,5,6
13	3,4'	67	2,3',4,5	121	2,3',4,5',6	174	2,2',3,3',4,5,6'
14	3,5	68	2,3',4,5'	122	2',3,3',4,5	175	2,2',3,3',4,5',6
15	4,4'	69	2,3',4,6	123	2',3,4,4'5	176	2,2',3,3',4,6,6'
Trichloro		70	2,3',4',5	124	2',3,4,5,5'	177	2,2',3,3',4',5,6
16	2,2',3	71	2,3',4',6	125	2',3,4,5,6'	178	2,2',3,3',5,5',6
17	2,2',4	72	2,3',5,5'	126	3,3',4,4',5	179	2,2',3,3',5,6,6'
18	2,2',5	73	2,3',5',6	127	3,3',4,5,5'	180	2,2',3,4,4',5,5'
19	2,2',6	74	2,4,4',5	Hexachloro		181	2,2',3,4,4',5,6
20	2,3,3'	75	2,4,4',6	128	2,2',3,3',4,4'	182	2,2',3,4,4',5,6'
21	2,3,4	76	2',3,4,5	129	2,2',3,3',4,5	183	2,2',3,4,4',5',6
22	2,3,4'	77	3,3',4,4'	130	2,2',3,3',4,5'	184	2,2',3,4,4',6,6'
23	2,3,5	78	3,3',4,5	131	2,2',3,3',4,6	185	2,2',3,4,5,5',6
24	2,3,6	79	3,3',4,5'	132	2,2',3,3',4,6'	186	2,2',3,4,5,6,6'
25	2,3',4	80	3,3',5,5'	133	2,2',3,3',5,5'	187	2,2',3,4',5,5',6
26	2,3',5	81	3,4,4',5	134	2,2',3,3',5,6	188	2,2',3,4',5,6,6'
27	2,3',6	Pentachloro		135	2,2',3'3',5,6'	189	2,3,3',4,4',5,5'
28	2,4,4'	82	2,2',3,3',4	136	2,2',3,3',6,6'	190	2,3,3',4,4',5,6
29	2,4,5	83	2,2',3,3',5	137	2,2',3,4,4',5	191	2,3,3',4,4',5',6
30	2,4,6	84	2,2',3,3',6	138	2,2',3,4,4',5'	192	2,3,3',4,5,5',6
31	2,4',5	85	2,2',3,4,4'	139	2,2',3,4,4',6	193	2,3,3',4',5,5',6
32	2,4',6	86	2,2',3,4,5	140	2,2',3,4,4',6'	Octachloro	
33	2',3,4	87	2,2',3,4,5'	141	2,2',3,4,5,5'	194	2,2',3,3',4,4',5,5'
34	2',3,5	88	2,2',3,4,6	142	2,2',3,4,5,6	195	2,2',3,3',4,4',5,6
35	3,3',4	89	2,2',3,4,6'	143	2,2',3,4,5,6'	196	2,2',3,3',4,4',5',6
36	3,3',5	90	2,2',3,4',5	144	2,2',3,4,5',6	197	2,2',3,3',4,4',6,6'
37	3,4,4'	91	2,2',3,4',6	145	2,2',3,4,6,6'	198	2,2',3,3',4,5,5',6
38	3,4,5	92	2,2',3,5,5'	146	2,2',3,4',5,5'	199	2,2',3,3',4,5,6,6'
39	3,4',5	93	2,2',3,5,6	147	2,2',3,4',5,6	200	2,2',3,3',4,5',6,6'
Tetrachloro		94	2,2',3,5,6'	148	2,2',3,4',5,6'	201	2,2',3,3',4',5,5',6
40	2,2',3,3'	95	2,2',3,5',6	149	2,2',3,4',5',6	202	2,2',3,3',5,5',6,6'
41	2,2',3,4	96	2,2',3,6,6'	150	2,2',3,4',6,6'	203	2,2',3,4,4',5,5',6
42	2,2',3,4'	97	2,2'3',4,5	151	2,2',3,5,5',6	204	2,2',3,4,4',5,6,6'
43	2,2',3,5	98	2,2',3',4,6	152	2,2',3,5,6,6'	205	2,3,3',4,4',5,5',6
44	2,2',3,5'	99	2,2',4,4',5	153	2,2',4,4',5,5'	Nonachloro	
45	2,2',3,6	100	2,2',4,4'6	154	2,2',4,4',5,6'	206	2,2',3,3',4,4',5,5',6
46	2,2',3,6'	101	2,2',4,5,5'	155	2,2',4,4',6,6'	207	2,2',3,3',4,4',5,6,6'
47	2,2',4,4'	102	2,2',4,5,6'	156	2,3,3',4,4',5	208	2,2',3,3',4,5,5',6,6'
48	2,2',4,5	103	2,2',4,5',6	157	2,3,3',4,4',5'	Decachloro	
49	2,2',4,5'	104	2,2',4,6,6'	158	2,3,3',4,4',6	209	2,2',3,3',4,4',5,5',6,6'
50	2,2',4,6	105	2,3,3',4,4'	159	2,3,3',4,5,5'		
51	2,2',4,6'	106	2,3,3',4,5	160	2,3,3',4,5,6		
52	2,2',5,5'						

Table III

Experimental retention times[17] and value of molecular descriptors* for PCBs

No 1**	RT(exp) 2	Cl(sq) 3	^{3D}W 4	$^{5}\chi_{pc}$ 5	$^{1}\chi^{v}$ 6	$^{4}\chi^{v}$ 7	No 1	RT(exp) 2	Cl(sq) 3	^{3D}W 4	$^{5}\chi_{pc}$ 5	$^{1}\chi^{v}$ 6	$^{4}\chi^{v}$ 7
1	0.1544	1	940.28	2.344	4.554	1.557	106	0.6680	25	986.43	5.167	6.479	2.538
2	0.1937	1	944.86	1.996	4.548	1.489	107	0.6628	25	986.68	4.625	6.473	2.437
3	0.1975	1	946.12	1.849	4.548	1.399	108	0.6626	25	987.04	5.102	6.473	2.626
4	0.2245	4	946.83	3.098	5.037	1.833	109	0.6016	25	982.65	5.453	6.479	2.792
5	0.2785	4	951.20	3.045	5.037	1.753	110	0.6314	25	982.48	4.969	6.479	2.485
6	0.2709	4	951.55	2.845	5.031	1.786	111	0.6183	25	985.62	4.868	6.467	2.710
7	0.2566	4	953.25	2.892	5.031	1.858	112	0.5986	25	980.96	5.188	6.661	2.809
8	0.2783	4	953.08	2.693	5.031	1.695	113	0.5862	25	981.45	5.217	6.473	2.759
9	0.257	4	951.61	2.724	5.031	1.734	114	0.6828	25	987.78	5.015	6.479	2.447
10	0.2243	4	947.42	3.403	5.037	1.993	115	0.6171	25	984.14	5.296	6.479	2.701
11	0.3238	4	956.22	2.492	5.025	1.716	116	0.6132	25	982.11	6.022	6.491	2.816
12	0.3298	4	957.75	2.494	5.031	1.604	117	0.6150	25	982.73	5.031	6.479	2.594
13	0.3315	4	957.32	2.345	5.025	1.626	118	0.6693	25	988.15	4.381	6.473	2.359
14	0.2973	4	956.03	2.732	5.025	1.876	119	0.5968	25	984.21	5.168	6.473	2.800
15	0.3387	4	959.35	2.199	5.025	1.536	120	0.6256	25	987.04	4.625	6.467	2.632
16	0.3625	9	958.22	3.807	5.520	2.030	121	0.5518	25	982.83	5.417	6.467	3.073
17	0.3398	9	959.68	3.647	5.514	2.134	122	0.6671	25	986.80	5.035	6.479	2.441
18	0.3378	9	958.39	3.484	5.514	2.011	123	0.6658	25	988.43	4.882	6.473	2.546
19	0.3045	9	954.39	4.077	5.520	2.248	124	0.6584	25	986.68	4.714	6.473	2.422
20	0.417	9	962.73	3.546	5.514	1.981	125	0.6142	25	982.77	5.404	6.479	2.682
21	0.4135	9	964.16	3.859	5.520	2.010	126	0.7512	25	992.83	4.473	6.473	2.290
22	0.4267	9	964.38	3.394	5.514	1.891	127	0.7078	25	991.13	4.711	6.467	2.562
23	0.377	9	962.58	3.625	5.514	2.094	128	0.7761	36	994.72	6.144	6.968	2.739
24	0.3508	9	958.57	3.964	5.520	2.141	129	0.7501	36	993.14	6.142	6.968	2.784
25	0.3937	9	964.41	3.394	5.508	2.086	130	0.7284	36	993.22	5.915	6.962	2.824
26	0.3911	9	962.76	3.226	5.508	1.963	131	0.6853	36	989.31	6.343	6.968	3.017
27	0.3521	9	958.93	3.910	5.514	2.222	132	0.7035	36	989.40	6.175	6.968	2.851
28	0.4031	9	965.83	3.242	5.508	1.995	133	0.6871	36	991.84	5.687	6.956	2.909
29	0.382	9	964.38	3.381	5.514	2.016	134	0.6796	36	988.03	6.086	6.968	2.911
30	0.3165	9	960.30	4.163	5.514	2.455	135	0.6563	36	987.81	5.951	6.962	2.937
31	0.4024	9	964.50	3.074	5.508	1.872	136	0.6257	36	984.73	6.133	6.968	2.943
32	0.3636	9	960.27	3.753	5.514	2.130	137	0.7329	36	993.87	5.982	6.962	2.887
33	0.4163	9	964.31	3.343	5.514	1.901	138	0.7403	36	993.99	5.664	6.962	2.746
34	0.3782	9	963.05	3.587	5.508	2.174	139	0.6707	36	990.92	6.176	6.962	3.120
35	0.4738	9	969.09	2.990	5.508	1.831	140	0.6707	36	990.98	6.367	7.133	3.365

Table III (Continued)

1	2	3	4	5	6	7	1	2	3	4	5	6	7
36	0.4375	9	967.56	3.228	5.502	2.103	141	0.7203	36	993.60	5.819	6.962	2.765
37	0.4858	9	970.81	2.843	5.088	1.550	142	0.6848	36	989.18	6.710	6.974	3.074
38	0.4593	9	968.64	3.479	5.514	1.948	143	0.6789	36	989.51	6.424	6.968	3.004
39	0.4488	9	969.10	3.081	5.502	2.013	144	0.6563	36	989.76	6.017	6.966	3.008
40	0.5102	16	969.37	4.516	6.003	2.227	145	0.6149	36	985.92	6.540	6.968	3.216
41	0.499	16	971.02	4.621	6.003	2.286	146	0.6955	36	992.66	5.435	6.956	2.831
42	0.487	16	971.13	4.356	5.997	2.33	147	0.6608	36	989.32	5.919	6.962	3.014
43	0.4587	16	969.41	4.393	5.997	2.371	148	0.6243	36	989.67	6.143	7.133	3.404
44	0.4832	16	969.44	4.193	5.997	2.208	149	0.6672	36	989.70	5.693	6.962	2.858
45	0.4334	16	965.67	4.645	6.003	2.398	150	0.5969	36	986.09	6.318	6.962	3.256
46	0.445	16	965.82	4.793	6.003	2.446	151	0.6499	36	988.01	5.760	7.102	3.012
47	0.4639	16	972.54	4.196	5.991	2.434	152	0.6062	36	984.35	6.290	6.968	3.110
48	0.4651	16	970.88	4.141	5.997	2.293	153	0.7036	36	995.57	5.184	6.956	2.752
49	0.461	16	971.09	4.033	5.991	2.311	154	0.6349	36	991.33	5.884	7.009	3.264
50	0.4007	16	967.31	4.837	5.997	2.711	155	0.5666	36	987.66	6.503	6.956	3.569
51	0.4242	16	967.31	4.033	5.991	2.311	156	0.8105	36	999.27	5.665	6.962	2.653
52	0.4557	16	969.61	3.869	5.991	2.189	157	0.8184	36	999.24	5.849	6.962	2.698
53	0.4187	16	965.84	4.467	5.913	2.356	158	0.7429	36	995.39	5.951	6.962	2.908
54	0.38	16	962.29	4.983	6.003	2.643	159	0.7655	36	998.00	5.909	6.879	2.834
55	0.5562	16	975.43	4.360	5.997	2.238	160	0.7396	36	993.65	6.529	6.968	3.045
56	0.5676	16	975.33	4.044	6.297	2.367	161	0.6968	36	994.24	6.199	6.956	3.181
57	0.5155	16	969.24	4.193	5.997	2.208	162	0.7737	36	997.75	5.615	6.956	2.782
58	0.5267	16	973.92	4.288	5.991	2.370	163	0.7396	36	993.70	5.686	6.962	2.801
59	0.486	16	969.99	4.471	5.997	2.370	164	0.7399	36	993.98	5.964	6.962	2.831
60	0.5676	16	976.97	4.208	5.997	2.147	165	0.6920	36	992.50	5.935	6.956	3.075
61	0.5331	16	974.86	4.666	6.003	2.310	166	0.7572	36	994.66	6.371	6.968	2.954
62	0.4685	16	971.25	4.946	6.003	2.563	167	0.7814	36	999.62	5.371	6.956	2.704
63	0.529	16	975.33	3.975	5.991	2.231	168	0.7068	36	995.57	6.163	6.956	3.145
64	0.4999	16	971.43	4.314	5.997	2.279	169	0.8625	36	1003.78	5.458	6.956	2.634
65	0.4671	16	969.67	4.682	6.003	2.457	170	0.8740	49	1006.08	6.956	7.451	3.040
66	0.5447	16	977.18	3.892	5.991	2.201	171	0.8089	49	1001.99	7.157	7.451	3.274
67	0.5214	16	975.56	3.883	5.991	2.244	172	0.8278	49	1004.29	6.727	7.445	3.125
68	0.504	16	975.80	4.136	5.985	2.474	173	0.8152	49	1000.11	7.426	7.457	3.271
69	0.451	16	971.70	4.670	5.991	2.684	174	0.7965	49	1000.64	6.992	7.451	3.153
70	0.5407	16	975.60	3.724	5.991	2.078	175	0.7611	49	1000.63	6.933	7.445	3.360
71	0.4989	16	971.46	4.408	5.997	2.337	176	0.7305	49	997.21	7.115	7.451	3.366
72	0.4984	16	973.94	3.967	5.985	2.351	177	0.8031	49	1000.62	6.900	7.451	3.168

Table III (Continued)

1	2	3	4	5	6	7	1	2	3	4	5	6	7
73	0.4554	16	970.20	4.657	5.991	2.611	178	0.7537	49	999.14	6.676	7.445	3.253
74	0.5341	16	977.03	3.731	6.078	2.166	179	0.7205	49	996.06	6.865	7.451	3.26
75	0.4643	16	972.91	4.513	5.991	2.593	180	0.8362	49	1006.20	6.476	7.445	3.046
76	0.5408	16	975.51	4.334	5.997	2.245	181	0.7968	49	1001.86	7.259	7.451	3.374
77	0.6295	16	981.66	3.488	5.991	1.946	182	0.7653	49	1001.81	7.184	7.445	3.466
78	0.6024	16	979.92	3.975	5.991	2.175	183	0.7720	49	1002.14	6.674	7.445	3.280
79	0.5894	16	980.15	3.726	5.985	2.218	184	0.7016	49	998.87	7.300	7.445	3.678
80	0.5464	16	978.68	3.964	5.979	2.490	185	0.7848	49	1000.56	7.100	7.451	3.252
81	0.6149	16	981.32	3.828	5.991	2.085	186	0.7416	49	997.27	7.630	7.457	3.470
82	0.6453	25	982.07	5.330	6.485	2.483	187	0.7654	49	1000.77	6.417	7.445	3.174
83	0.6029	25	980.57	5.101	6.479	2.568	188	0.6920	49	997.30	7.050	7.445	3.573
84	0.5744	25	976.91	5.361	6.485	2.595	189	0.9142	49	1010.31	6.656	7.445	2.998
85	0.6224	25	983.60	5.170	6.479	2.587	190	0.8740	49	1005.14	7.026	7.451	3.161
86	0.6105	25	981.89	5.433	6.485	2.587	191	0.8447	49	1005.83	6.946	7.445	3.253
87	0.6175	25	982.38	5.007	6.479	2.464	192	0.8269	49	1004.90	7.275	7.445	3.434
88	0.5486	25	978.39	5.627	6.485	2.820	193	0.8397	49	1005.08	6.682	7.445	3.146
89	0.5779	25	977.99	5.607	6.485	2.702	194	0.9620	64	1016.87	7.768	7.934	3.341
90	0.5814	25	982.24	4.941	6.473	2.672	195	0.9321	64	1013.18	8.241	7.940	3.527
91	0.5549	25	978.58	5.194	6.479	2.698	196	0.8938	64	1013.26	7.974	7.934	3.575
92	0.5742	25	980.62	4.778	6.473	2.549	197	0.8293	64	1010.15	8.097	7.934	3.788
93	0.5437	25	976.60	5.370	6.485	2.714	198	0.8845	64	1011.92	8.017	7.934	3.613
94	0.5331	25	976.69	5.383	6.479	2.788	199	0.8494	64	1008.41	8.205	7.940	3.620
95	0.5464	25	976.97	5.035	6.479	2.576	200	0.8197	64	1008.52	7.847	7.934	3.683
96	0.5057	25	973.65	5.558	6.485	2.793	201	0.8875	64	1011.69	7.717	7.934	3.469
97	0.61	25	981.32	4.850	6.479	2.489	202	0.8089	64	1006.85	7.597	7.934	3.577
98	0.5415	25	978.27	5.553	6.479	2.908	203	0.8938	64	1013.39	7.758	7.934	3.534
99	0.588	25	983.90	4.690	6.473	2.593	204	0.8217	64	1009.79	8.390	7.934	3.933
100	0.5212	25	980.21	5.386	6.473	3.011	205	0.9678	64	1017.32	8.022	7.934	3.506
101	0.5816	25	982.21	4.527	6.473	2.471	206	1.0103	81	1024.01	9.057	8.423	3.829
102	0.5431	25	978.59	5.124	6.479	2.709	207	0.9423	81	1020.71	9.187	8.423	4.042
103	0.5142	25	978.68	5.227	6.473	2.890	208	0.9320	81	1019.34	8.937	8.423	3.937
104	0.4757	25	975.10	5.743	6.479	3.106	209	1.0496	100	1031.62	10.277	9.076	4.526
105	0.7049	25	988.17	4.858	6.479	2.353							

* Abbreviation used are shown in Table 1; ** The number of each PCB[9]

Table IV
Experimental and predicted RRT of Polychlorinated biphenyls

	Relative Retention Times				
		Predicted RRT			
No*	Exp.**	Eqn. 5	Eqn. 6	Eqn. 8	Eqn. 9
1	0.1544	0.1439	0.1292	0.1375	0.0831
2	0.1937	0.1953	0.1714	0.1887	0.1272
3	0.1975	0.2093	0.1923	0.2027	0.1508
4	0.2245	0.2173	0.2169	0.2106	0.1625
5	0.2785	0.2656	0.2748	0.2588	0.2228
6	0.2709	0.2695	0.2620	0.2627	0.2091
7	0.2566	0.2882	0.2709	0.2813	0.2158
8	0.2783	0.2863	0.2858	0.2794	0.2355
9	0.2570	0.2702	0.2650	0.2633	0.2136
10	0.2243	0.2238	0.2126	0.2171	0.1535
11	0.3238	0.3207	0.3052	0.3136	0.2543
12	0.3298	0.3374	0.3411	0.3302	0.2935
13	0.3315	0.3327	0.3244	0.3256	0.2762
14	0.2973	0.3186	0.2890	0.3116	0.2334
15	0.3387	0.3547	0.3537	0.3475	0.3082
16	0.3625	0.3425	0.3613	0.3353	0.3011
17	0.3398	0.3583	0.3507	0.3511	0.2874
18	0.3378	0.3443	0.3487	0.3372	0.2891
19	0.3045	0.3007	0.2976	0.2937	0.2309
20	0.4170	0.3912	0.4041	0.3839	0.3453
21	0.4135	0.4066	0.4317	0.3992	0.3721
22	0.4267	0.4089	0.4290	0.4015	0.3729
23	0.3770	0.3896	0.3877	0.3823	0.3256
24	0.3508	0.3463	0.3548	0.3391	0.2913
25	0.3937	0.4093	0.3962	0.4019	0.3343
26	0.3911	0.3915	0.3900	0.3842	0.3318
27	0.3521	0.3502	0.3418	0.3430	0.2759
28	0.4031	0.4245	0.4187	0.4170	0.3596
29	0.3820	0.4089	0.4073	0.4015	0.3475
30	0.3165	0.3650	0.3310	0.3578	0.2582
31	0.4024	0.4102	0.4160	0.4028	0.3605
32	0.3636	0.3647	0.3634	0.3575	0.3003
33	0.4163	0.4082	0.4238	0.4008	0.3674
34	0.3782	0.3947	0.3769	0.3873	0.3124
35	0.4738	0.4592	0.4682	0.4516	0.4139
36	0.4375	0.4429	0.4182	0.4354	0.3558
37	0.4858	0.4774	0.4976	0.4698	0.4517
38	0.4593	0.4544	0.4701	0.4468	0.4123
39	0.4488	0.4593	0.4422	0.4517	0.3825
40	0.5102	0.4622	0.4965	0.4546	0.4305
41	0.4990	0.4797	0.5101	0.4720	0.4423
42	0.4870	0.4808	0.4894	0.4731	0.4203
43	0.4587	0.4626	0.4658	0.4550	0.3955
44	0.4832	0.4629	0.4829	0.4553	0.4174
45	0.4334	0.4228	0.4346	0.4153	0.3635
46	0.4450	0.4244	0.4360	0.4169	0.3635
47	0.4639	0.4957	0.4783	0.4880	0.4061
48	0.4651	0.4782	0.4815	0.4705	0.4135
49	0.4610	0.4804	0.4746	0.4727	0.4060
50	0.4007	0.4403	0.4096	0.4327	0.3292
51	0.4242	0.4403	0.4336	0.4327	0.3651
52	0.4557	0.4647	0.4703	0.4571	0.4054
53	0.4187	0.4246	0.4279	0.4171	0.3581
54	0.3800	0.3865	0.3748	0.3792	0.2965
55	0.5562	0.5261	0.5516	0.5182	0.4852
56	0.5676	0.5251	0.5325	0.5172	0.4623
57	0.5155	0.4608	0.4807	0.4532	0.4153
58	0.5267	0.5103	0.5089	0.5024	0.4386
59	0.4860	0.4688	0.4764	0.4611	0.4062
60	0.5676	0.5422	0.5755	0.5343	0.5118
61	0.5331	0.5201	0.5500	0.5123	0.4815
62	0.4685	0.4821	0.4833	0.4744	0.4073
63	0.5290	0.5251	0.5308	0.5172	0.4647
64	0.4999	0.4840	0.4990	0.4763	0.4314
65	0.4671	0.4654	0.4700	0.4577	0.3971
66	0.5447	0.5444	0.5515	0.5365	0.4862
67	0.5214	0.5275	0.5263	0.5196	0.4597
68	0.5040	0.5300	0.5033	0.5221	0.4299
69	0.4510	0.4869	0.4524	0.4791	0.3728
70	0.5407	0.5279	0.5461	0.5200	0.4845
71	0.4989	0.4843	0.4945	0.4766	0.4252
72	0.4984	0.5105	0.4948	0.5026	0.4251
73	0.4554	0.4710	0.4477	0.4633	0.3703
74	0.5341	0.5428	0.5531	0.5349	0.4889
75	0.4643	0.4996	0.4725	0.4918	0.3956
76	0.5408	0.5269	0.5499	0.5191	0.4833
77	0.6295	0.5910	0.6213	0.5829	0.5636
78	0.6024	0.5730	0.5899	0.5649	0.5254
79	0.5894	0.5753	0.5716	0.5673	0.5058
80	0.5464	0.5601	0.5222	0.5520	0.4484
81	0.6149	0.5875	0.6124	0.5793	0.5506
82	0.6453	0.5952	0.6376	0.5871	0.5640
83	0.6029	0.5797	0.5945	0.5716	0.5184
84	0.5744	0.5416	0.5646	0.5337	0.4876
85	0.6224	0.6110	0.6278	0.6028	0.5511
86	0.6105	0.5934	0.6237	0.5852	0.5470
87	0.6175	0.5984	0.6266	0.5903	0.5535
88	0.5486	0.5570	0.5570	0.5490	0.4734
89	0.5779	0.5529	0.5714	0.5449	0.4913
90	0.5814	0.5970	0.5863	0.5888	0.5070
91	0.5549	0.5590	0.5561	0.5510	0.4761
92	0.5742	0.5802	0.5807	0.5721	0.5051
93	0.5437	0.5384	0.5417	0.5304	0.4613

Table IV (Continued)

No*	Exp.**	Eqn. 5	Eqn. 6	Eqn. 8	Eqn. 9
94	0.5331	0.5393	0.5306	0.5314	0.4479
95	0.5464	0.5422	0.5507	0.5343	0.4743
96	0.5057	0.5074	0.5065	0.4996	0.4237
97	0.6100	0.5875	0.6026	0.5793	0.5288
98	0.5415	0.5558	0.5366	0.5478	0.4504
99	0.5880	0.6141	0.6041	0.6059	0.5273
100	0.5212	0.5760	0.5310	0.5679	0.4417
101	0.5816	0.5967	0.5977	0.5885	0.5244
102	0.5431	0.5591	0.5506	0.5511	0.4703
103	0.5142	0.5601	0.5263	0.5520	0.4406
104	0.4757	0.5226	0.4791	0.5148	0.3870
105	0.7049	0.6579	0.7000	0.6495	0.6302
106	0.6680	0.6401	0.6665	0.6318	0.5913
107	0.6628	0.6427	0.6570	0.6343	0.5847
108	0.6626	0.6464	0.6545	0.6380	0.5766
109	0.6016	0.6012	0.5982	0.5930	0.5154
110	0.6314	0.5995	0.6221	0.5913	0.5484
111	0.6183	0.6318	0.6122	0.6235	0.5318
112	0.5986	0.5837	0.5753	0.5756	0.4920
113	0.5862	0.5888	0.5778	0.5807	0.4960
114	0.6828	0.6539	0.6883	0.6456	0.6158
115	0.6171	0.6166	0.6212	0.6084	0.5411
116	0.6132	0.5957	0.6193	0.5875	0.5358
117	0.6150	0.6021	0.6098	0.5939	0.5329
118	0.6693	0.6577	0.6730	0.6493	0.6031
119	0.5968	0.6173	0.5982	0.6091	0.5151
120	0.6256	0.6464	0.6277	0.6380	0.5497
121	0.5518	0.6031	0.5502	0.5949	0.4591
122	0.6671	0.6439	0.6798	0.6356	0.6074
123	0.6658	0.6606	0.6713	0.6522	0.5958
124	0.6584	0.6427	0.6642	0.6343	0.5924
125	0.6142	0.6025	0.6153	0 5943	0.5358
126	0.7512	0.7053	0.7402	0.6967	0.6723
127	0.7078	0.6881	0.6884	0.6795	0.6124
128	0.7761	0.7244	0.7717	0.7157	0.6905
129	0.7501	0.7084	0.7469	0.6998	0.6644
130	0.7284	0.7092	0.7286	0.7006	0.6449
131	0.6853	0.6696	0.6770	0.6611	0.5876
132	0.7035	0.6705	0.6969	0.6620	0.6124
133	0.6871	0.6953	0.6869	0.6867	0.6006
134	0.6796	0.6565	0.6673	0.6481	0.5810
135	0.6563	0.6543	0.6530	0.6459	0.5659
136	0.6257	0.6227	0.6287	0.6144	0.5414
137	0.7329	0.7158	0.7286	0.7072	0.6430
138	0.7403	0.7170	0.7367	0.7084	0.6553
139	0.6707	0.6859	0.6679	0.6774	0.5754
140	0.6707	0.6865	0.6492	0.6780	0.5494
141	0.7203	0.7131	0.7375	0.7045	0.6555
142	0.6848	0.6682	0.6859	0.6598	0.5948
143	0.6789	0.6716	0.6857	0.6631	0.5966
144	0.6563	0.6741	0.6659	0.6657	0.5768
145	0.6149	0.6349	0.6174	0.6266	0.5220
146	0.6955	0.7036	0.6954	0.6950	0.6115
147	0.6608	0.6697	0.6547	0.6612	0.5653
148	0.6243	0.6732	0.6165	0.6648	0.5156
149	0.6672	0.6735	0.6730	0.6651	0.5882
150	0.5969	0.6366	0.6003	0.6283	0.5038
151	0.6499	0.6563	0.6419	0.6479	0.5526
152	0.6062	0.6188	0.6049	0.6105	0.5127
153	0.7036	0.7330	0.7269	0.7242	0.6453
154	0.6349	0.6901	0.6358	0.6816	0.5391
155	0.5666	0.6527	0.5742	0.6443	0.4684
156	0.8105	0.7700	0.8095	0.7612	0.7309
157	0.8184	0.7697	0.8114	0.7609	0.7314
158	0.7429	0.7311	0.7399	0.7224	0.6537
159	0.7655	0.7573	0.7727	0.7485	0.6887
160	0.7396	0.7136	0.7292	0.7050	0.6389
161	0.6968	0.7195	0.6944	0.7109	0.6001
162	0.7737	0.7548	0.7684	0.7460	0.6859
163	0.7396	0.7141	0.7255	0.7055	0.6424
164	0.7399	0.7169	0.7383	0.7083	0.6543
165	0.6920	0.7020	0.6793	0.6934	0.5882
166	0.7572	0.7238	0.7470	0.7151	0.6594
167	0.7814	0.7735	0.7887	0.7647	0.7086
168	0.7068	0.7330	0.7129	0.7242	0.6197
169	0.8625	0.8149	0.8502	0.8058	0.7721
170	0.8740	0.8376	0.8776	0.8285	0.7874
171	0.8089	0.7971	0.8047	0.7882	0.7076
172	0.8278	0.8199	0.8314	0.8109	0.7387
173	0.8152	0.7784	0.7995	0.7695	0.7026
174	0.7965	0.7837	0.8016	0.7748	0.7081
175	0.7611	0.7836	0.7632	0.7747	0.6636
176	0.7305	0.7494	0.7353	0.7406	0.6355
177	0.8031	0.7835	0.7940	0.7746	0.7001
178	0.7537	0.7687	0.7514	0.7599	0.6549
179	0.7205	0.7379	0.7273	0.7291	0.6307
180	0.8362	0.8388	0.8520	0.8296	0.7616
181	0.7968	0.7958	0.7919	0.7869	0.6919
182	0.7653	0.7953	0.7716	0.7864	0.6688
183	0.7720	0.7986	0.7792	0.7897	0.6820
184	0.7016	0.7660	0.7103	0.7572	0.6013
185	0.7848	0.7829	0.7899	0.7740	0.6935
186	0.7416	0.7500	0.7462	0.7412	0.6433
187	0.7654	0.7850	0.7685	0.7761	0.6744
188	0.6920	0.7503	0.6976	0.7415	0.5917
189	0.9142	0.8791	0.9141	0.8698	0.8252
190	0.8740	0.8283	0.8508	0.8192	0.7571

Table IV (Continued)

No*	Exp.**	Eqn. 5	Eqn. 6	Eqn. 8	Eqn. 9
191	0.8447	0.8351	0.8382	0.8260	0.7417
192	0.8269	0.8260	0.8152	0.8169	0.7134
193	0.8397	0.8277	0.8340	0.8186	0.7407
194	0.9620	0.9428	0.9708	0.9332	0.8717
195	0.9321	0.9071	0.9251	0.8977	0.8206
196	0.8938	0.9079	0.9033	0.8984	0.7973
197	0.8293	0.8775	0.8404	0.8683	0.7281
198	0.8845	0.8948	0.8847	0.8855	0.7776
199	0.8494	0.8605	0.8559	0.8513	0.7486
200	0.8197	0.8616	0.8271	0.8524	0.7179
201	0.8875	0.8926	0.8905	0.8832	0.7876
202	0.8089	0.8452	0.8136	0.8360	0.7075
203	0.8938	0.9091	0.9002	0.8997	0.7954
204	0.8217	0.8740	0.8278	0.8647	0.7112
205	0.9678	0.9471	0.9614	0.9376	0.8575
206	1.0103	1.0112	1.0122	1.0014	0.8987
207	0.9423	0.9797	0.9477	0.9700	0.8278
208	0.9320	0.9666	0.9372	0.9569	0.8204
209	1.0496	1.0830	1.0246	1.0729	0.8905

* The number of each PCB is according Ref. 9; **Ref. 17

Table V
Multiple regression coefficients and statistical data for model 2

	Equation 6	Equation 9
	Coefficient	Coefficient
Constant	-10.2229 (± 0.1856)	-10.3289 (± 0.9163)
^{3D}W	0.0108 (±0.0002)	0.0112 (±0.0001)
$^{4}\chi^{v}$	-0.1678 (± 0.0062)	-0.1975 (± 0.0410)
$^{5}\chi^{pc}$	0.0531 (± 0.0032)	0.0751 (± 0.0207)
Cl (sq.)	-0.0033 (± 0.0002)	-0.0021 (± 0.0008)
$^{1}\chi^{v}$	0.0680 (±0.0079)	0.0187 (±0.0375)
s	0.0104	0.0119
F	12263	1678
Df	5, 203	5, 15
R^2	0.9967	0.9982
N	209	21
MAE	0.0081	0.0083
DW	1.2727	1.8273

Table VI
Multiple regression coefficients and statistical data for model 2

	^{3D}W	$^{4}\chi^{v}$	$^{5}\chi^{pc}$	Cl (sq.)	$^{1}\chi^{v}$
^{3D}W	1.000				
$^{4}\chi^{v}$	0.879	1.000			
$^{5}\chi^{pc}$	0.915	0.975	1.000		
Cl (sq.)	0.549	0.935	0.967	1.000	
$^{1}\chi^{v}$	0.969	0.953	0.975	0.976	1.000

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