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GAS CHROMATOGRAPHIC DATA FOR CHLOROBENZENES, CHLOROANILINES AND N-SULPHINYLANILINES

RELATIONSHIP BETWEEN MOLECULAR STRUCTURE AND RETENTION BASED ON RETENTION INDEX INCREMENTS CALCULATED BY COMPUTER

Z. CZERWIEC
Department of Chemistry, Pedagogical University, Czestochowa (Poland)
and
M. V. BUDAHEGYI and J. M. TAKÁCS*
Gas Chromatographic Research Group for Study of Retention Index Systems, Fábián utca 27, 1165-Budapest (Hungary)

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SUMMARY

The relationship between molecular structure and retention based on retention index increments using chlorobenzenes, chloroanilines and N-sulphinylanilines was investigated. Calculations and coding of the individual bonds were performed by computer.

INTRODUCTION

Some of the most important gas–liquid chromatographic studies in recent years are those dealing with the problems of molecular structure and gas chromatographic retention. It is not our purpose to review publications in this area, as we have mentioned the most important in our previous papers on this topic[1–3].

In this paper, the most significant problems of the relationship between molecular structure and gas chromatographic retention are dealt with only in relation to retention index increments. As the basis of our approach relying on bond energy and/or bond distance was discussed in detail in a previous paper[3], we shall not repeat it here.

As we have been studying aromatic sulphinylanilines[4,5], we considered using these compounds, which have interesting structures, as model materials for simplifying and further developing our previous, complicated computer method of molecular structure examination.

Beagley *et al.*[6], Van Woerden and Bijl-Vlieger[7] and Janelli *et al.*[8] have published thermodynamic data on compounds of similar types; however, most of these data could not be used for our purposes as the primary and/or, more frequently, the

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secondary environment of the bonds of these compounds[9] differed from those of the substances with which we were concerned. Therefore, other practicable thermodynamic data were sought, and were found in papers by Martin and Kiss[10], Huggins[11], Skancke[12], Jug and Bussian[13], Hirota *et al.*[14] and Kiss and Szöke[15], primarily in the form of bond orders.

THEORETICAL

Based on the concept of retention index increments, the following equation can be written for isothermal and constant gas chromatographic conditions:

$$I^{\text{st.ph.}}_{\text{substance}}(T) = I_a + I_b + I^{\text{st.ph.}}_i(T) \tag{1}$$

where

I = the isothermal retention index, in index units (i.u.);
st.ph. = stationary phase;
T = column temperature (°K or °C);
I_a = atomic index contribution (i.u.):

$$I_a = \frac{\text{molecular weight}}{10} \tag{2}$$

I_b = bond index contribution (i.u.):

$$I_b = \sum_{n=1}^{m} i_b(n) \tag{3}$$

n = serial number of increments in the molecule;
m = number of increments in the molecule;
i_b = bond increment value (i.u.);
I_i = interaction index contribution (i.u.):

$$I^{\text{st.ph.}}_i(T) = \sum_{n=1}^{m} i_i\,(\text{st.ph.}, T, n) \tag{4}$$

i_i = interaction increment value (i.u.).

For describing the atoms in the molecule, the notion of an atomic code number was introduced. The atomic code number is a three-figure number of the general form xyz. The meanings of the individual digits are as follows.

The value of x represents the character of the chemical bond (aromatic, triple bond, etc.) in which the atom takes part. Considering that a polybasic atom, *e.g.*, carbon, can form bonds of various kinds simultaneously, the chemical bonds were classified as single, double, triple and aromatic. In this classification, the value of the arrangement increases from left to right. In all instances, the bond that is arranged at a higher level in the classification should be coded as x. The code digits for the different chemical bonds are as follows: 1 = single bond; 2 = double bond; 3 = triple bond; 4 = aromatic bond.

The value of y refers to the quality of the atom. The code digits are as follows: 1 = first-order carbon atom; it should be noted that "order" in the classical sense is meant, namely, the number of other carbon atoms to which the carbon atom in question is linked; 2 = second-order carbon atom; 3 = third-order carbon atom; 4 = fourth-order carbon atom; 5 = oxygen atom; 6 = nitrogen atom; 7 = hydrogen atom; 8 = sulphur atom; 9 = chlorine atom. At the present stage of our research it was not appropriate to develop a general code system containing all atoms, but the use of y = 5–9 allows the system to be extended to a few atoms other than carbon.

The value of z denotes the position occupied by the atom in the molecule examined. The code numbers are as follows: 0 = atom in the molecular skeleton (chain, ring, etc.); 1 = atom linked directly to the skeleton; 2 = atom linked to an atom that is directly connected with the molecular skeleton; 3 = some other position.

The atomic code numbers of the atoms in the molecule are coded visually, for small molecules, by means of the so-called atomic code network. For large molecules (naphthalene derivatives, steroids, etc.) it is expedient to perform the coding by computer. In the present work, the code network in Fig. 1 was used. It should be noted that this network is also suitable for coding other molecules with structures similar to those of the compounds examined (anilines, benzene derivatives, etc.).

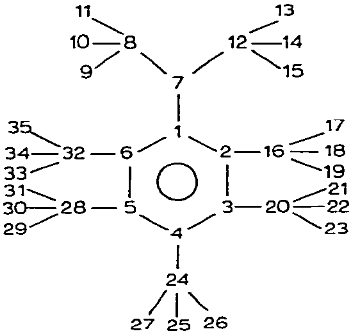


Fig. 1. Code network used for coding the compounds examined.

The code network contains 35 atoms. Thus, the individual atomic places of the network are given in the form of $P(k)$, where k indicates the serial number of the atom in the network. Among the 35 atoms, 35 chemical bonds may be produced theoretically in the cases examined; therefore, all possible forms of these should be given in a general form to the computer. Denoting the individual bonds by $B(k)$, these are as follows: $B(1) = P(1) - P(2)$; $B(2) = P(2) - P(3)$; $B(3) = P(3) - P(4)$; $B(4) = P(4) - P(5)$; $B(5) = P(5) - P(6)$; $B(6) = P(1) - P(6)$; $B(7) = P(1) - P(7)$; $B(8) = P(7) - P(8)$; $B(9) = P(8) - P(9)$; $B(10) = P(8) - P(10)$; $B(11) = P(8) - P(11)$; $B(12) = P(7) - P(12)$; $B(13) = P(12) - P(13)$; $B(14) = P(12) - P(14)$; $B(15) = P(12) - P(15)$; $B(16) = P(2) - P(16)$; $B(17) = P(16) - P(17)$; $B(18) = P(16) - P(18)$; $B(19) = P(16) - P(19)$; $B(20) = P(3) - P(20)$; $B(21) = P(20) - P(21)$; $B(22) = P(20) - P(22)$; $B(23) = P(20) - P(23)$; $B(24) = P(4) - P(24)$; $B(25) = P(23) - P(24)$; $B(26) = P(24) - P(25)$; $B(27) = P(24) - P(26)$; $B(28) = P(5) - P(28)$; $B(29) = P(28) - P(29)$; $B(30) = P(28) - P(30)$; $B(31) = P(28) - P(31)$; $B(32) = P(6) - P(32)$; $B(33) = P(32) - P(33)$; $B(34) = P(32) - P(34)$; $B(35) = P(32) - P(35)$.

Frequently in the course of practical work the compound examined contains no atom at the individual atomic places of the conceptual code network, and in this instance $P(k) = 0$ there. In such a case, all $B(k)$ values "theoretically" containing the atom in question are, of course, zero.

Coding rules for chemical bonds

(1) The code of a chemical bond starts by the atomic code number of two atoms between which the bond has been formed. In the first position is the atomic code number with a lower number value. The two atomic code numbers are separated from each other by a hyphen and after the second atomic code number there is a colon.

(2) After the colon closing the atomic codes of the atoms taking part in the bond, the primary and then the secondary environments of the atom in the first position should be coded, following in each instance the order of increasing number. The code of the complete environment of the first atom is closed by a semi-colon; thus $B(3, 2)$ = 430-430:171-430, 171-430.91;.

(3) The code numbers of the atoms belonging to the environment of the other atom taking part in the bond should be written as a new line below the codes of the environment of the first atom. The individual environments are separated from each other by a comma, and between the individual atomic code numbers is a hyphen. The complete bond code is closed by a full stop:

$B(3, 2)$ = 430-430: 171-430, 171-430.91;
171-430.91, 191-430.61.

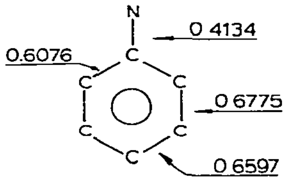
(4) It frequently occurs that the atomic code numbers of two atoms taking part in the bond are identical. In such a case, the order is decided by the primary, secondary, etc., environment. In all instances, the atom having an environment with a lower number is given first.

(5) If a heteroatom is bonded to the one being examined, then the quality and position of this bond should be given as a decimal of the atomic code number of the atom being examined. With the examined compounds, for example, a nitrogen atom is bonded to the C(1) carbon atom, so the atomic code number of the C(1) atom is 430.61. If more than one heteroatom is bonded to the atom being examined, then the data for these should be given in increasing numerical order, as decimals, together with the atomic code number of the atom being examined. With the N-sulphinylanilines, for example, a nitrogen and an oxygen atom are bonded to the sulphur atom, so the atomic code number of the sulphur atom is 282.5361.

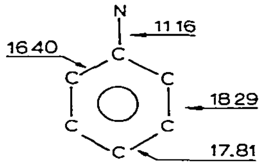
(6) After the full stop closing the complete code of the chemical bond, the value of the increment should be given in index units with an accuracy of two decimals, denoting generally the data bank serial number of the compound, as well as the serial number of the increment in the molecule: $B(32,7) = 18.75$ i.u.

The introduction of the three-figure atomic code numbers (xyz), in addition to the shaping of increment codes and bond codes depending on them by adapting suitable increment values, has created a wide-ranging research basis for investigations related to molecular structure which was not possible before. The system developed permits an unambiguous description of the relationships among the various physical and chemical properties of the molecular structure and the molecule.

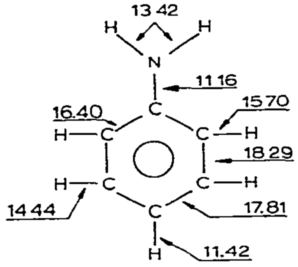
An example is given of the calculation of bond increment values where bond orders are used as a basis for calculation. According to Kiss and Szöke[15], the bond orders of aniline are as follows:



With this bond order, 116.15 i.u. was obtained by gas chromatographic data. As the sum of the bond orders is 4.3030, a value corresponding to a bond order of unity could be calculated, and was 26.99 i.u. By means of the latter, the corresponding bond increment values could easily be calculated:



Combining the data obtained from the bond orders with our data obtained previously, the complete bond increment system for aniline could be written:



Summarizing the bond increment values of aniline, the value of the bond index contribution is obtained as 214.70 i.u. As the molecular weight of the aniline is 93.00, the atomic index contribution is 9.30 i.u. As

$$I_M = I_a + I_b \tag{5}$$

where I_M is the molecular index contribution (i.u.), the molecular index contribution of aniline is

$$I_M(\text{aniline}) = 9.30 + 214.70 = 224.00 \text{ i.u.} \tag{6}$$

The calculation of the interaction index increment values using 10% (w/w) SE-30 as stationary phase at 180.0°C, where the retention index of the aniline is 986.0 i.u., can be given. From eqn. 1:

$$I_{i,\mathrm{aniline}}^{10\%(\mathrm{w/w})\mathrm{SE\text{-}30}}\ (180.0°\mathrm{C}) = 986.0 - 224.0 = 762.0\ \mathrm{i.u.} \tag{7}$$

Assuming a practically homogeneous distribution of the interactions in the molecule, which can of course be realized only approximately in reality because of orientation effects and other reasons, we can write

$$I_b{:}I_i = i_b(n){:}i_i(n) \tag{8}$$

For example, let us calculate the interaction increment value for a C–N bond in aniline using 10% (w/w) SE-30 as the stationary phase at 180.0°C:

$$214.70{:}762.0 = 11.16{:}i_i(\mathrm{C{-}N}) \tag{9}$$

$$i_i(\mathrm{C{-}N}) = \frac{762.0}{214.7} \cdot 11.16 = 39.61\ \mathrm{i.u.} \tag{10}$$

As the bond index contribution and/or the bond increment value do not depend on the stationary phase used or on the column temperature, it is possible to study the dependence of the interaction increment value on column temperature. Using Váradi and Tóth's[16] experimental data, Table I shows the temperature dependence of the interaction increment (C–N) between the C–N bond of aniline using PEG 20M as the stationary phase.

TABLE I

CHANGES IN THE INTERACTION INCREMENT [i_i(C–N)] ON PEG 20M AS STATIONARY PHASE WITH COLUMN TEMPERATURE

Column temperature (°C)	*Interaction increment [i_i(C–N)]*
100	76.79
120	77.66
140	78.61
160	79.44
180	80.83
200	82.13

EXPERIMENTAL

The measurements necessary for the calculations were performed on a Varian 2860 gas chromatograph with a flame-ionization detector. Nitrogen was used as the carrier gas, hydrogen and air as auxiliary gases. Calibrations were carried out using a Hamilton syringe with an *n*-alkane mixture. The column was a 50 m × 1.0 mm I.D. stainless-steel capillary WCOT with OS-138 as the stationary phase. The optimal flow-rate of the carrier gas was 5.0 ml/min. The column temperature was 180.0°C and the evaporation temperature was 200°C.

For the calculations, a Hewlett-Packard 9830A computer with a complementary memory unit and a Hewlett-Packard 9866A printer were used. The programs were written in Basic. A block diagram of the program is shown in Fig. 2.

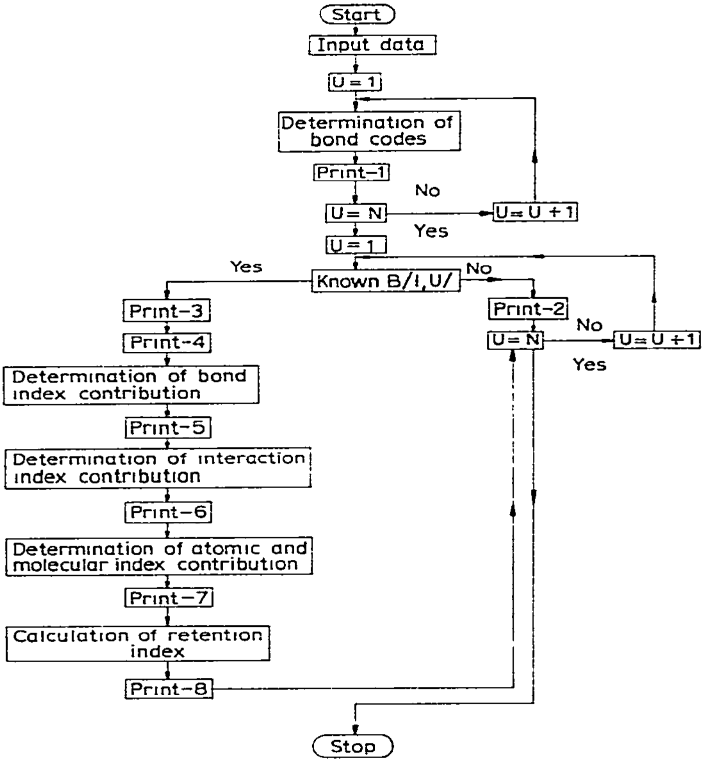


Fig. 2. Block diagram of the computer program.

In our case, the input data were as follows:

(a) Serial number of the compound examined:

0: benzene;
1: aniline;
2: 2,6-dichlorosulphinylaniline;
3: 3,5-dichlorosulphinylaniline;
4: 3,4-dichlorosulphinylaniline;
5: 2,3-dichlorosulphinylaniline;
6: 2,4-dichlorosulphinylaniline;
7: 2,5-dichlorosulphinylaniline;
8: *o*-chloroaniline;
9: *m*-chloroaniline;
10: *p*-chloroaniline;
11: chlorobenzene;
12: *o*-dichlorobenzene;
13: *m*-dichlorobenzene;

14: *p*-dichlorobenzene;
15: 2,6-dichloroaniline;
16: 2,4-dichloroaniline;
17: 2,5-dichloroaniline;
18: 2,3-dichloroaniline;
19: 3,5-dichloroaniline;
20: 1,2,3-trichlorobenzene;
21: 1,2,4-trichlorobenzene;
22: 1,3,5-trichlorobenzene;
23: 1,2,3,5-tetrachlorobenzene;
24: 1,2,4,5-tetrachlorobenzene.

(b) Number of compounds to be examined (N = 24).
(c) Molecular weight of the compounds examined.
(d) Increment values.
(e) Stationary phase (s).
(f) Column temperature (s).

The labelling used on the computer block diagram was as follows:

PRINT-1: Codes of the compound bonds without increment values.

PRINT-2: The calculation cannot be performed owing to lack of data.

PRINT-3: Bond codes of the compound with bond increment values.

PRINT-4: Bond codes of the compound with interaction increment values on given stationary phase at the given column temperature.

PRINT-5: I_b value.

PRINT-6: I_i value.

PRINT-7: I_a and I_M values.

PRINT-8: Retention index of the compound examined on the given stationary phase at the given column temperature.

TABLE II

BOND INCREMENT VALUES OF THE COMPOUNDS EXAMINED

Bond code symbol	*Increment value (i.u.)*	*Identities*
$B(8.1)$	13.42	$B(8,10)$, $B(12,10)$, $B(12,1)$, $B(8,19)$, $B(8,9)$, $B(12,9)$, $B(12,19)$
$B(8,8)$	13.46	$B(12,8)$, $B(8,16)$, $B(8,17)$, $B(8,18)$, $B(12,16)$, $B(12,17)$, $B(12,18)$
$B(8,15)$	13.48	$B(12,15)$
$B(7,1)$	11.16	$B(7,10)$
$B(7,9)$	11.24	
$B(7,19)$	12.65	
$B(7,8)$	13.08	$B(7,16)$
$B(7,18)$	13.56	
$B(7,17)$	13.80	
$B(7,15)$	13.86	
$B(7,4)$	14.28	
$B(7,3)$	14.20	
$B(7,6)$	13.98	

TABLE II *(continued)*

Bond code symbol	*Increment value (i.u.)*	*Identities*
B(7,5)	14.00	
B(7,7)	14.09	
B(7,2)	13.75	
B(7,11)	17.33	*B*(7,14), *B*(24,10), *B*(24,14)
B(20,9)	17.28	*B*(28,17)
B(24,6)	17.23	*B*(24,16), *B*(24,21), *B*(7,13), *B*(20,13)
B(28,7)	17.13	
B(20,3)	17.32	
B(28,19)	17.38	*B*(20,19)
B(7,22)	17.45	*B*(28,22), *B*(28,23), *B*(20,22)
B(16,7)	16.02	
B(16,2)	16.06	
B(16,8)	16.15	*B*(16,17)
B(32,15)	16.00	*B*(16,15)
B(16,16)	16.03	
B(16,6)	16.04	
B(7,12)	16.30	*B*(7,21)
B(24,4)	18.56	*B*(7,20), *B*(20,20)
B(20,5)	18.05	*B*(20,18)
B(20,4)	17.98	
B(16,21)	16.38	*B*(7,24), *B*(16,24). *B*(24,24), *B*(28,24)
B(7,23)	16.36	*B*(20,23)
B(16,18)	16.38	
B(16,5)	16.41	
B(16,20)	16.30	*B*(16,23)
B(24,1)	11.42	*B*(32,0), *B*(28,0), *B*(24,0), *B*(20,0), *B*(16,0), *B*(7,0)
B(20,1)	14.44	*B*(28,1), *B*(28,8)
B(20,11)	11.35	*B*(24,8), *B*(24,12), *B*(28,12)
B(28,5)	23.46	*B*(28,18), *B*(28,9)
B(24,2)	19.07	*B*(28,13), *B*(28,20), *B*(24,15)
B(16,1)	15.70	*B*(32,1), *B*(32,9)
B(32,18)	15.00	*B*(32,8)
B(32,5)	22.54	
B(32.10)	22.50	*B*(16,10)
B(32,16)	22.52	
B(32,4)	22.54	
B(32,6)	22.56	
B(16,11)	11.25	*B*(28,9), *B*(24,9), *B*(24,13), *B*(32,13)
B(20,2)	19.00	*B*(20,8), *B*(28,15). *B*(20,15)
B(24,5)	24.08	*B*(32,12), *B*(24,18), *B*(20,12), *B*(24,20), *B*(32,20)
B(28,6)	19.00	*B*(20,10), *B*(28,10), *B*(28,16)
B(28,4)	19.15	
B(28,21)	11.20	*B*(16,14)
B(20,7)	19.55	*B*(20,17)

(Continued on p. 56)

TABLE II *(continued)*

Bond code symbol	*Increment value (i.u.)*	*Identities*
$B(24,7)$	24.10	$B(16,14)$, $B(24,17)$
$B(32,21)$	23.92	
$B(16,9)$	24.02	$B(32,19)$, $B(16,19)$
$B(32,17)$	22.06	
$B(16,3)$	18.75	
$B(16,4)$	18.85	
$B(32,7)$	18.75	
$B(24,3)$	22.80	$B(16,22)$, $B(16,13)$, $B(24,19)$, $B(24,22)$, $B(32,22)$
$B(20,6)$	22.86	$B(20,16)$
$B(20,21)$	22.90	$B(32,23)$, $B(24,23)$
$B(20,24)$	22.94	$B(32,24)$
$B(1,0)$	14.39	$B(2,0)$, $B(3,0)$, $B(4,0)$, $B(5,0)$, $B(6,0)$
$B(3,1)$	17.81	$B(4,1)$
$B(3,11)$	20.61	
$B(2,1)$	18.29	$B(5,1)$
$B(5,8)$	24.46	
$B(2,11)$	20.87	
$B(3,8)$	24.11	
$B(3,12)$	23.78	$B(5,12)$
$B(4,8)$	24.45	
$B(4,9)$	25.19	
$B(4,5)$	23.82	$B(4,18)$
$B(4,12)$	22.96	
$B(5,9)$	25.20	
$B(5,18)$	25.97	
$B(4,13)$	20.73	$B(5,13)$
$B(3,2)$	22.87	$B(3,15)$, $B(4,15)$
$B(4,20)$	24.41	$B(5,20)$
$B(5,5)$	24.37	
$B(2,10)$	24.10	$B(5,10)$
$B(5,16)$	24.10	
$B(5,4)$	24.12	
$B(5,6)$	24.12	
$B(2,10)$	26.74	$B(5,14)$, $B(2,14)$
$B(3,7)$	24.15	$B(3,17)$
$B(5,21)$	23.57	
$B(1,1)$	16.40	$B(6,1)$
$B(6,9)$	23.55	
$B(6,8)$	22.86	
$B(6,18)$	27.24	
$B(6,5)$	25.16	
$B(1,10)$	21.72	$B(6,10)$
$B(6,16)$	25.00	
$B(6,4)$	26.03	
$B(6,6)$	25.16	
$B(1,9)$	22.19	
$B(6,19)$	25.40	$B(1,19)$
$B(6,17)$	23.60	
$B(1,3)$	24.79	
$B(6,7)$	25.51	
$B(1,4)$	26.17	

TABLE II *(continued)*

Bond code symbol	*Increment value (i.u.)*	*Identities*
B(1,11)	19.82	
B(3,9)	24.84	
B(3,13)	22.01	*B*(6,13)
B(2,8)	24.22	
B(5,15)	22.25	*B*(2,15)
B(2,2)	23.50	
B(2,12)	23.30	*B*(6,12)
B(3,5)	22.59	*B*(3,18)
B(3,20)	26.91	*B*(6,20)
B(3,10)	22.68	*B*(4,10)
B(4,6)	23.02	*B*(4,16)
B(4,4)	23.43	
B(1,14)	25.00	*B*(3,14), *B*(4,14), *B*(6,14)
B(4,7)	22.90	*B*(4,17)
B(4,21)	24.65	
B(2,17)	24.20	
B(2,7)	23.50	
B(6,21)	24.70	
B(2,9)	24.95	
B(5,19)	25.81	*B*(2,19)
B(5,17)	24.72	
B(2,3)	23.14	
B(2,4)	24.94	
B(5,7)	23.81	
B(1,9)	22.31	*B*(1,13), *B*(2,13)
B(3,3)	22.43	*B*(3,19)
B(1,22)	21.97	*B*(2,22), *B*(3,22), *B*(4,22), *B*(5,22), *B*(6,22)
B(2,16)	23.70	
B(2,6)	23.90	
B(2,21)	25.05	
B(3,6)	23.37	
B(3,16)	25.99	
B(3,21)	24.53	
B(3,19)	26.01	*B*(4,19)
B(4,23)	29.15	*B*(5,23)
B(2,24)	29.72	
B(3,23)	29.23	*B*(6,23)
B(1,8)	21.54	
B(1,16)	24.00	
B(1,18)	26.06	
B(1,17)	24.10	
B(1,15)	22.00	*B*(6,15)
B(1,5)	24.24	
B(1,7)	25.47	
B(1,2)	23.70	
B(1,6)	25.66	
B(3,4)	22.55	
B(1,12)	21.12	
B(1,21)	21,64	
B(2,18)	25.10	
B(1,20)	27.19	*B*(2,20)
B(1,24)	29.11	*B*(4,24)
B(2,5)	22.44	
B(1,23)	28.03	*B*(2,23)

TABLE III

COMPARISON OF MEASURED AND CALCULATED RETENTION INDICES

*Compound**	*Gas chromatographic parameters*	*Retention index (i.u.)*		
		Measured	*Calculated*	*Difference*
2,3-Cl$_2$SA	OS-138/180°C	1876	1873	+3
2,4-Cl$_2$SA	OS-138/180°C	1844	1845	−1
2,5-Cl$_2$SA	OS-138/180°C	1836	1835	+1
2,6-Cl$_2$SA	OS-138/180°C	1764	1764	0
3,4-Cl$_2$SA	OS-138/180°C	1855	1857	−2
3,5-Cl$_2$SA		1803	1805	−2
o-ClA	OV-7/100°C	1203 (ref. 17)	1200	+3
m-ClA	OV-7/100°C	1281 (ref. 17)	1278	+3
p-ClA	OV-7/100°C	1282 (ref. 17)	1279	+3
ClB	Apiezon L/130°C	885	885	0
2,6-Cl$_2$A	OS-138/180°C	1601	1605	−4
2,4-Cl$_2$A	OS-138/180°C	1717	1716	+1
2,5-Cl$_2$A	OS-138/180°C	1717	1716	+1
2,3-Cl$_2$A	OS-138/180°C	1746	1743	+3
3,5-Cl$_2$A	OS-138/180°C	1813	1808	+5
o-Cl$_2$B	OV-225/100°C	1309 (ref. 17)	1307	+2
m-Cl$_2$B	OV-225/100°C	1245 (ref. 17)	1242	+3
p-Cl$_2$B	OV-225/100°C	1264 (ref. 17)	1262	+2
1,2,3-Cl$_3$B	OV-225/100°C	1501 (ref. 17)	1499	+2
1,2,4-Cl$_3$B	OV-225/100°C	1441 (ref. 17)	1439	+2
1,3,5-Cl$_3$B	OV-225/100°C	1344 (ref. 17)	1341	+3
1,2,3,5-Cl$_4$B	OV-225/100°C	1565 (ref. 17)	1563	+2
1,2,4,5-Cl$_4$B	OV-225/100°C	1583 (ref. 17)	1580	+3

* S = sulphinyl; A = aniline; B = benzene.

Table II gives the increment values of the compounds examined, and the measured and calculated retention indices of the compounds examined are listed in Table III.

REFERENCES

1 J. Takács, C. Szita and G. Tarján, *J. Chromatogr.*, 56 (1971) 1.
2 T. S. Lombosi, E. R. Lombosi, I. Bernát, Zs. Sz. Bernát, E. C. Takács and J. M. Takács, *J. Chromatogr.*, 119 (1976) 307.
3 I. Fisch, I. Olácsi, M. Richter, A. P. Sinka, E. C. Takács, J. M. Takács, J. Vörös and G. Tarján, *J. Chromatogr.*, 148 (1978) 17.
4 Z. Czerwiec and J. Markowski, *J. Chromatogr.*, 124 (1976) 76.
5 Z. Czerwiec, *J. Chromatogr.*, 139 (1977) 177.
6 B. Beagley, S. J. Chantrell, R. G. Kirby and D. G. Schmidling, *J. Mol. Struct.*, 25 (1975) 319.
7 H. F. van Woerden and S. H. Bijl-Vlieger, *Rec. Trav. Chim. Pays-Bas*, 93 (1974) 85.
8 L. Janelli, U. Lamanna and H. Lumbroso, *Bull. Chim. Soc. Fr.*, (1966) 3626.
9 M. Budahegyi, T. Lombosi, E. Lombosi, S. Mészáros, ifj. Sz. Nyiredy, G. Tarján, J. Vörös and J. Takács, *Magy. Kém. Foly.*, 85 (1979) 292.
10 A. Martin and A. I. Kiss, *Acta Chim. Acad. Sci. Hung.*, 91 (1976) 105.
11 M. L. Huggins, *J. Amer. Chem. Soc.*, 75 (1953) 4123.
12 A. Skancke, *J. Mol. Struct.*, 42 (1977) 235.
13 K. Jug and B. M. Bussian, *Theor. Chim. Acta*, 50 (1978) 1.
14 M. Hirota, T. Iijima and M. Kimura, *Bull. Chem. Soc. Jap.*, 51 (1978) 1589.
15 A. I. Kiss and J. Szöke, *Quantum Spectroscopy*, KFKI, Budapest, 1972, No. 4, p. 1.
16 A. Váradi and T. Tóth, *Magy. Kém. Foly.*, 80 (1974) 41.
17 S. D. West and R. C. Hall, *J. Chromatogr. Sci.*, 13 (1975) 5.