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# Prediction of the gas chromatographic retention values of chlorobenzenes on different stationary phases by using structure–retention correlations

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## Abstract

The retention values (capacity factors or retention indices) of the isomers of chlorobenzenes with two to six chlorine atoms were predicted by using structure–retention correlations and the calculated contributions of the *ortho*, *meta* and *para* positions of the substituent atoms on the aromatic ring. The method permits the prediction of the retention of every isomer by starting from the measured retention of a few compounds, and does not require the use of all of the possible isomers as standard samples for the identification in complex mixtures. © 1998 Elsevier Science Ltd

**Keywords:** Retention indices; Retention factor; Retention prediction; Structure–retention relationships; Chlorobenzenes

## 1. Introduction

The prediction of the retention values of organic compounds by using structure–retention correlation is of great interest because it can allow to foresee the elution order of molecules belonging to various homologous series when authentic standards are not available. Such a procedure is more attractive than the prediction of retention values by starting from the tabulated or measured values of the physical properties (boiling points, density, molecular volume, etc.), because only structural data and a few experimental measurement of the gas chromatographic retention of selected reference compounds are necessary.

Many papers have been published on the correla-

tion between physical properties and retention values of chemical compounds: linear, branched and cyclic alkanes, alkenes and alkadienes [1–14]; alcohols [10,12,13,15,16]; alkyl iodides [17–20] and other halogenated compounds [2,20–33]; alkylbenzenes [9,12,34–41] and other aromatic compounds with different substituent groups [12,22–26,30,32,35,37,41–43]. Some of these papers propose methods for the prediction of retention values on the basis of structural considerations. The behaviour of aromatic compounds was studied both from the point of view of properties–retention [9,12,13,22,39,40,42] and structure–retention [2,9,12,13,23,25,35–37,39–41] correlations. The retention values of chlorobenzenes were predicted by correlation with molar heat, enthalpy and entropy of solution [22], as a function of the number of chlorine atoms in the molecule at different temperatures [37], with topologically based incremental models [43], and by

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using the difference in retention index between the isomers as a function of temperature [24,35].

In papers published previously [30,32–34] some of us considered the correlations between structure and retention of chlorobenzenes on different capillary columns. In this paper, a method is described which allows the prediction of retention times of all of the chlorobenzenes by using only a few experimental values as the starting data, and consideration of the *ortho*, *meta* or *para* positions of the chlorine atoms on the aromatic ring. Similar methods can be applied to aromatic compounds with other substituent groups.

## 2. Method of prediction

In the method used, the structure of each of the possible poly-chlorobenzenes can be obtained by adding one to five chlorine atoms in different positions to the precursor molecule: chlorobenzene. By addition of a second chlorine atom, the isomers of dichlorobenzene are formed: 1,2-dichlorobenzene, 1,3-dichlorobenzene and 1,4-dichlorobenzene when the addition is in the *ortho*, *meta* or *para* position, respectively. The additions of a third and of a fourth chlorine atom lead to the formation of the three possible trichlorobenzenes and tetrachlorobenzenes, where *ortho*, *meta* and *para* correlations are simultaneously present when every chlorine atom is considered with respect to the other.

As the addition of the various chlorine atoms in different positions leads to different increments of the retention time of the isomer compound with respect to the precursor chlorobenzene, a numerical value can be correlated to each *ortho*, *meta* or *para* substitution. The value of this 'effect' can be expressed by using various retention data (adjusted retention data,  $t'_R$ , retention volumes or retention indices). For a theoretically rigorous treatment, the best parameter is the capacity factor  $k' = t'_R/t_M$  where  $t_M$  is the dead time or gas hold-up time of the column under the conditions (temperature, carrier gas, flow-rate) used for the analysis. In fact,  $k'$  is correlated with the partition coefficient of the solute–solvent pair, and is therefore characteristic of the liquid phase and of the compound analysed. The retention index values,  $I$ , obtained with the classical

Kovats equation, can also be used. However, as  $I$  depends on the retention of both the analysed compound and of the reference  $n$ -alkane homologous series, the numerical values of the *ortho*, *meta* and *para* effects obtained by using  $I$  values ( $O_I$ ,  $M_I$ ,  $P_I$ ) are valid only for the stationary phase used. On the other hand, the use of  $I$  values measured on similar columns, and those taken from the literature, allows to calculate the  $O_I$ ,  $M_I$ ,  $P_I$  effects of a given column and to predict the  $I$  values without experimentally measuring the retention times of all of the isomers.

## 3. Experimental

In this paper a method employing the  $k'$  values is described in detail: the differences  $\Delta \ln k'_i$  between the  $\ln k'_i$  of each isomer and the  $\ln k'_1$  of the chlorobenzene are used as a measure of the change of retention of a given isomer with  $n$  chlorine atoms with respect to the mono-substituted chlorobenzene.

Table 1 shows the retention values measured experimentally on two capillary column and the values of  $\ln k'$  and  $\Delta \ln k'_i$ . Fused-silica capillary columns, 30 m×0.32 mm I.D. and 0.25  $\mu\text{m}$  film thickness were used: DB-5 (stationary phase, 5% diphenyl–95% dimethylpolysiloxane), from J&W Scientific (Folsom, CA, USA) and BPX-70 (stationary phase, 70% cyanopropyl–polysilphenylene–siloxane) from SGE (Ringwood, Australia). These two stationary phases were selected as the DB-5 has a constant polarity within a wide temperature range, with a  $\Delta C$  value of 2.72 [44–46], whereas the BPX-70 column shows a  $\Delta C$  changing from 7.33 to 8.67 in the temperature range 60–180°C. (The  $\Delta C$  is the difference in apparent carbon number of linear alkanes and alcohols with the same retention, used as a polarity parameter for the classification of stationary phases, which evaluates the influence of the hydrogen bonds and dipole moments with respect of purely dispersion interactions. Its value for liquid phases ranges from 1.5 for non polar squalane to about 9 for highly polar BPX-70. For some phases its values depend on temperature (see Refs. [44–46]).)

The procedure used for the calculation of the O, M and P effects can be explained by taking into account, as an example, the compound 1,2,3-tri-

Table 1

Experimental values of  $t'_R$ ,  $\ln k'_i$  and  $\Delta \ln k'_i$  of all chlorobenzenes measured on DB-5 and BPX-70 columns: temperature 100°C, carrier gas helium, flow-rate 63.5 cm/s

Compound	DB-5 column			BPX-70 column		
	$t'_R$	$\ln k'_i$	$\Delta \ln k'_i$	$t'_R$	$\ln k'_i$	$\Delta \ln k'_i$
Chlorobenzene	0.448	-0.565	0.000	0.272	-1.064	0.000
1,2-Dichlorobenzene	1.254	0.465	1.030	0.905	0.139	1.203
1,3-Dichlorobenzene	1.059	0.296	0.861	0.615	-0.248	0.817
1,4-Dichlorobenzene	1.093	0.328	0.892	0.700	-0.118	0.946
1,2,3-Trichlorobenzene	3.485	1.487	2.052	2.440	1.131	2.195
1,2,4-Trichlorobenzene	2.836	1.281	1.846	1.660	0.746	1.810
1,3,5-Trichlorobenzene	2.189	1.022	1.587	0.905	0.139	1.203
1,2,3,4-Tetrachlorobenzene	8.877	2.422	2.987	5.444	1.933	2.998
1,2,3,5-Tetrachlorobenzene	6.711	2.143	2.708	3.114	1.375	2.439
1,2,4,5-Tetrachlorobenzene	6.768	2.151	2.716	3.310	1.436	2.500
Pentachlorobenzene	19.500	3.209	3.774	8.939	2.429	3.494
Hexachlorobenzene	53.671	4.222	4.787	22.563	3.355	4.420

chlorobenzene. In this molecule, two *ortho* effects are simultaneously present between the two chlorine atoms in positions 1 and 2 and between those in 2 and 3. At the same time, a *meta* effect exists between the atoms in 1 and 3 positions. The influence on the retention of *ortho* and *meta* effects in a molecule of trichlorobenzene ( $O_3$  and  $M_3$ ) is different from that of the same effect in the simpler dichlorobenzene isomers ( $O_2$  and  $M_2$ ), because of the modifying influence of the third chlorine atom. We can therefore write an equation where the numerical values of the  $O_3$  and  $M_3$  effects for a trichlorobenzene molecule are correlated with the increment of retention of the given isomer with respect of the precursor molecule with one chlorine atom. The equation for 1,2,3-trichlorobenzene is:

$$2O_3 + M_3 = (\ln k'_{123} - \ln k'_1) = \Delta \ln k'_{123} \quad (1)$$

where  $\ln k'_{123}$  and  $\ln k'_1$  are, respectively, the natural logarithms of the capacity factors of 1,2,3-trichlorobenzene and of chlorobenzene, and  $\Delta \ln k'_{123}$  is the difference between these values.

A general numerical equation can be obtained, which correlates the *ortho*, *meta* and *para* effects with the capacity factors:

$$\alpha_i O_n + \beta_i M_n + \gamma_i P_n = \Delta \ln k'_i \quad (2)$$

where the coefficients  $\alpha_i$ ,  $\beta_i$  and  $\gamma_i$  are the number of *ortho*, *meta* and *para* effects simultaneously present in the selected isomer  $i$ , and  $O_n$ ,  $M_n$  and  $P_n$  are the values of the *ortho*, *meta* and *para* contributions

characteristic of the isomers with  $n$  chlorine atoms. It is supposed that the values of  $O_n$ ,  $M_n$  and  $P_n$  do not change when isomers with the same number  $n$  of chlorine atoms are considered, i.e. that the differences due to the relative position of the substituent are negligible with respect to the average value of the *ortho*, *meta* and *para* effects for a given  $n$ . As shown below, this hypothesis was found to be justified. When Eq. (2) is applied to a series of isomers with the same  $n$  value, systems of three equations with three unknowns are obtained. As an example, when  $n=2$  we obtain:

$$O_2 = \Delta \ln k'_{12} \quad \text{only one } \textit{ortho} \text{ effect for 1,2-dichlorobenzene} \quad (3)$$

$$M_2 = \Delta \ln k'_{13} \quad \text{only one } \textit{meta} \text{ effect for 1,3-dichlorobenzene} \quad (4)$$

$$P_2 = \Delta \ln k'_{14} \quad \text{only one } \textit{para} \text{ effect for 1,4-dichlorobenzene} \quad (5)$$

where  $\alpha_{12}=1$ ,  $\beta_{13}=1$ ,  $\gamma_{14}=1$  and all other coefficients ( $\beta_{12}$ ,  $\gamma_{12}$ ,  $\alpha_{13}$ ,  $\gamma_{13}$ ,  $\alpha_{14}$ ,  $\beta_{14}$ ) are equal to zero. When the isomers with three chlorine atoms are considered, the following system is obtained:

$$2O_3 + M_3 = \Delta \ln k'_{123} \quad \text{for 1,2,3-trichlorobenzene} \quad (6)$$

$$O_3 + M_3 + P_3 = \Delta \ln k'_{124}$$

for 1,2,4-trichlorobenzene (7)

$$3M_3 = \Delta \ln k'_{135}$$

for 1,3,5-trichlorobenzene (8)

In fact, two *ortho* effects are present in 1,2,3-trichlorobenzene between the chlorine atoms in position 1 vs. 2 and 2 vs. 3, whereas the *meta* effect is between position 1 and 3; again 1,2,4-trichlorobenzene exhibits one *ortho* effect between position 1 and 2, one *meta* effect between position 2 and 4, and one *para* effect between position 1 and 4; 1,3,5-trichlorobenzene exhibits three *meta* effects between positions 1 and 3, 3 and 5, and 1 and 5.

By applying the same rule to tetra-, penta- and hexachlorobenzene, we obtain:

$$3O_4 + 2M_4 + P_4 = \Delta \ln k'_{1234} \quad (9)$$

$$2O_4 + 2M_4 + 2P_4 = \Delta \ln k'_{1245} \quad (10)$$

$$2O_4 + 3M_4 + P_4 = \Delta \ln k'_{1235} \quad (11)$$

$$4O_5 + 4M_5 + 2P_5 = \Delta \ln k'_{\text{penta}} \quad (12)$$

$$6O_6 + 6M_6 + 3P_6 = \Delta \ln k'_{\text{hexa}} \quad (13)$$

The solution of the systems with three equations and three unknowns shown in Eqs. (3)–(5), Eqs. (6)–(8) and Eqs. (9)–(11) can be easily obtained with standard procedures. The results obtained by applying the above listed equations to the experimental retention data shown in Table 1 are reported in Table 2.

Table 2

Values of O, M and P effects as a function of the number of chlorine atoms,  $n$ , calculated with Eqs. (3)–(13) by using experimental values shown in Table 1 for DB-5 and BPX-70 columns

$n$	DB-5 column			BPX-70 column		
	O	M	P	O	M	P
2	1.030	0.861	0.892	1.203	0.817	0.946
3	0.762	0.529	0.555	0.897	0.401	0.512
4	0.636	0.357	0.365	0.769	0.210	0.271
5	0.554	0.257	0.265	0.689	0.103	0.163
6	0.505	0.193	0.198	0.646	0.043	0.095

It has been observed that by using the experimental values of  $k'$  obtained with many columns, the numerical values of the O, M and P effects follow a linear behaviour on a three-dimension graph (see Fig. 1), where the experimental values of O, M and P shown in Table 2 for the DB-5 column are plotted on the three axes *ortho*, *meta* and *para*. This means that, by plotting P and M as a function of O, straight lines are also obtained on the plots P vs. O and M vs. O. The calculation of the coefficients of the equation on three dimensions can, therefore, be replaced by the simple determination of the slope coefficients,  $m$ , and of the intercepts,  $q$ , of the straight lines on the P vs. O and M vs. O plots, which is possible by using only two experimental points.

$$M_n = m_M O_n + q_M \quad (14)$$

$$P_n = m_P O_n + q_P \quad (15)$$

by replacing these values into Eq. (2) we obtain:

$$\alpha_i O_n + \beta_i (m_M O_n + q_M) + \gamma_i (m_P O_n + q_P) = \Delta \ln k'_i \quad (16)$$

$$O_n = \frac{\Delta \ln k'_i - \beta_i q_M - \gamma_i q_P}{\alpha_i + \beta_i m_M + \gamma_i m_P} \quad (17)$$

The values of  $M_n$  and  $P_n$  are obtained by replacing the  $O_n$  value obtained with Eq. (17) into Eq. (14) and Eq. (15). Of course, the plots P vs. M and O vs. M, or M vs. P and O vs. P, can be considered with the same results.

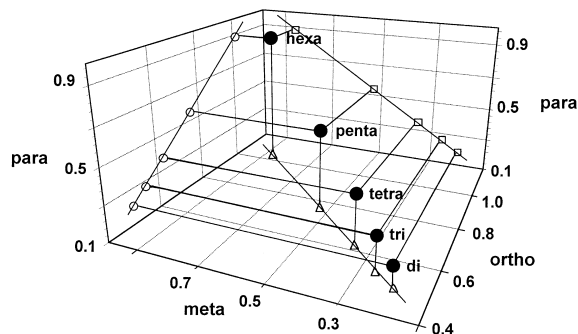


Fig. 1. Three-dimensional graph showing the straight-line behaviour of *ortho*, *meta* and *para* effects for chlorobenzenes with different numbers of chlorine atoms analysed on the DB-5 column. The projections on the three planes P vs. M, O vs. M and P vs. O are also shown.

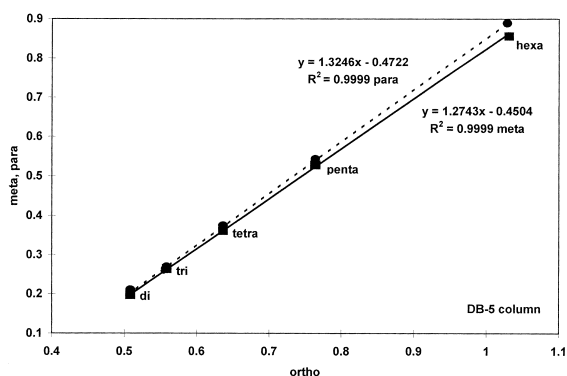


Fig. 2. Straight-line behaviour of *para* (upper line) and *meta* (lower line) effects as a function of the *ortho* effect on the DB-5 column.

The *ortho*, *meta* and *para* effects were calculated. Figs. 2 and 3 show that for both columns, on the M vs. O and P vs. O plots, their values for di-, tri and tetrachlorobenzene follow a straight line. It is therefore possible to predict the O, M and P values of compounds with  $n$  from 2 to 4 without solving the corresponding system of equations but simply interpolating the straight lines with coefficients  $m_M$ ,  $m_P$ ,  $q_M$  and  $q_P$  obtained with two sets of O, M and P values (e.g. using the data of di- and tetrachlorobenzenes to obtain those of trichlorobenzenes).

With this procedure it is also possible to obtain the O, M and P values for penta- and hexachlorobenzene. In fact, Eqs. (12) and (13) cannot be solved, because the systems of equations used for isomers with a smaller  $n$  value cannot be written. As the

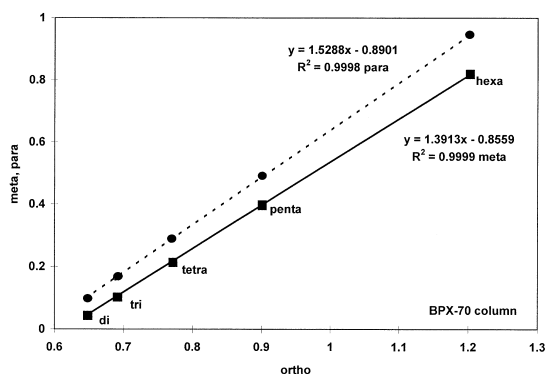


Fig. 3. Straight-line behaviour of *para* (upper line) and *meta* (lower line) effects as a function of the *ortho* effect on the BPX-70 column.

values of O, M and P follow a straight line relationship, it is reasonable to expect that the O, M and P effects for penta- and hexachlorobenzene lie on the same line, and the  $M_5$ ,  $M_6$ ,  $P_5$  and  $P_6$  values can be obtained by placing the values of  $O_5$  and  $O_6$ , respectively, in the equation obtained with a least-squares best-fit procedure on the M vs. O and P vs. O plots. Table 2 shows the values of the effects O, M and P on the two columns, DB-5 and BPX-70. By using these values in the equation previously seen, the  $k'$  of every chlorobenzene can be obtained, and the retention time calculated. Fig. 4 shows the flow diagram of the procedure used for the calculation,

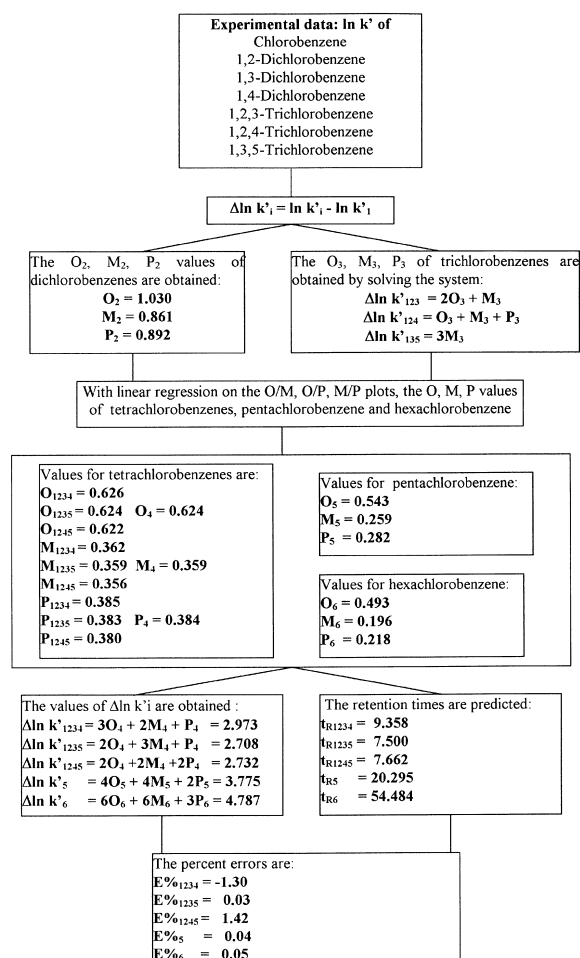


Fig. 4. Flow diagram of the procedure used for the prediction of tetra-, penta- and hexachlorobenzenes by starting from experimental retention of di- and trichlorobenzenes on DB-5.

Table 3

Predicted values of  $t'_R$ ,  $\ln k'$  and  $\Delta \ln k'$  of all chlorobenzenes measured on DB-5 and BPX-70 columns at a temperature of 100°C

Compound	Equation	DB-5 column			BPX-70 column		
		$\Delta \ln k'_i$	$\ln k'_i$	$t'_R$	$\Delta \ln k'_i$	$\ln k'_i$	$t'_R$
1,2-Dichlorobenzene	O	1.030	0.465	1.254	1.203	0.139	0.905
1,3-Dichlorobenzene	M	0.861	0.296	1.059	0.817	-0.248	0.615
1,4-Dichlorobenzene	P	0.892	0.328	1.093	0.946	-0.118	0.700
1,2,3-Trichlorobenzene	2O+M	2.052	1.487	3.485	2.195	1.131	2.440
1,2,4-Trichlorobenzene	O+M+P	1.846	1.281	2.836	1.810	0.746	1.660
1,3,5-Trichlorobenzene	3M	1.587	1.022	2.189	1.203	0.139	0.905
1,2,3,4-Tetrachlorobenzene	3O+2M+P	2.986	2.421	8.868	2.998	1.934	5.444
1,2,3,5-Tetrachlorobenzene	2O+3M+P	2.707	2.142	6.706	2.439	1.375	3.114
1,2,4,5-Tetrachlorobenzene	2O+2M+2P	2.715	2.151	6.763	2.500	1.436	3.310
Pentachlorobenzene	4O+4M+2P	3.774	3.210	19.501	3.494	2.429	8.938
Hexachlorobenzene	6O+6M+3P	4.787	4.222	53.670	4.420	3.355	22.562

with, as example, the prediction of retention times of tetra-, penta- and hexachlorobenzenes by starting from experimental retention of di- and trichlorobenzenes on DB-5.

Table 3 shows the calculated values of  $k'$  and  $t'_R$  for all of the chlorobenzenes, analysed at 100°C on the DB-5 and BPX-70 columns. The differences between experimental (see Table 1) and calculated  $t'_R$  values are very small (average percent error 0.02% on DB-5 and 0.01% on BPX-70), and the method can therefore be used for the prediction of the retention of every isomer with two to six chlorine atoms, when a small number of compounds, suitable for the solution of the equation shown, is available. The good correspondence between experimental and calculated values confirms the hypothesis that the  $O_i$ ,

$M_i$  and  $P_i$  effects depend only on the number of chlorine atoms and not on the isomer considered. The last box of Fig. 4 shows the percent errors between experimental and calculated values for the various isomers, due to the choice of the starting data (retention of di- and trichlorobenzenes) selected for this example.

Table 4 shows the errors observed when the experimental retentions of different isomers are used as the starting values for the prediction of the retention of other compounds on a DB-5 column. The fitting between experimental and predicted values depends on the linearity of the values of the effects O, M and P on the three-dimensional space (see Fig. 1). When only tetra-, penta- or hexachlorobenzenes are used as starting compounds, the accura-

Table 4

Percent errors observed when the experimental retentions of different isomers are used as the starting values for the prediction of the retention of the other compounds on DB-5 column

Analysed isomers	% error on the predicted retention of the various isomers										
	12	13	14	123	124	135	1234	1235	1245	5	6
di + tri							-1.30	0.03	1.42	0.04	0.05
di + tetra				0.86	-0.74	-0.67				0.01	0.06
di + penta				-0.17	-0.18	-0.18	-1.30	0.03	1.42		0.05
di + hexa				-0.17	-0.18	-0.18	-1.30	0.03	1.42	0.04	
tri + tetra	0.00	-0.56	-0.56							0.07	0.03
tri + penta	0.00	-0.58	-0.59				-1.31	0.03	1.41		0.05
tri + hexa	0.00	-0.58	-0.59				-1.30	0.03	1.42	0.04	
tetra + penta	0.00	-0.62	-0.69	4.20	-2.29	-2.00					0.15
tetra + hexa	0.01	-0.61	-0.65	3.09	-1.82	-1.59				0.02	
penta + hexa	0.00	-0.58	-0.59	-0.17	-0.18	-0.18	-1.30	0.03	1.42		

Table 5

Values of  $O_i$ ,  $M_i$  and  $P_i$  effects as a function of the number of chlorine atoms,  $n$ , calculated for dichlorobenzenes from experimental data on an SPB-1 column; for trichlorobenzene from literature data on an SE-30 column predicted for tetrachlorobenzenes

$n$	$O_i$	$M_i$	$P_i$	Data
2	201.0	175.0	178.0	Experimental
3	139.8	103.3	105.8	Literature
4	109.8	68.1	70.4	Predicted

cy of the prediction is lower, but it is good enough to allow the prediction of the retention of compounds not available as standard samples. The same behaviour was observed with other columns. The same procedure can be used with other series of isomers, such as chlorobenzoamines, chlorophenols, etc.

If the retention index values,  $I$ , are used instead of the  $k'$  values, the procedure can be applied by using literature data which list the  $I$  values on the same or similar columns. As discussed in Section 1, the  $O_i$ ,  $M_i$  and  $P_i$  values are only valid for the given stationary phase, and cannot be used to compare the behaviour of different stationary phases on a common basis, because the  $I$  values depend on the solute–solvent interaction of both the analysed compounds and the reference  $n$ -alkane series. However, owing to the great number of  $I$  values available in the literature, the suggested method can help in the identification of compounds belonging to different series of substituted benzenes.

One can take, as an example, the prediction of the  $I$  values of tetrachlorobenzenes on a capillary bonded phase column filled with polydimethylsiloxane (SPB-1, 30 m×0.32 mm I.D., 0.25 μm film thickness, Supelco, Bellefonte, PA, USA), by using as the starting data the  $I$  values of mono- and dichlorobenzenes experimentally measured on the same column, and the  $I$  values of trichlorobenzenes taken from the literature [24] and measured on a column (25 m×0.22 mm I.D.) wall-coated with SE-30 methylsilicone (SGE, Australia). The dimensions of the columns are different, but the chemical composition of the liquid phase is the same (all-*methyl*-substituted polysiloxane). The  $I$  values at 140°C were used in both instances. Table 5 shows the  $O_i$ ,  $M_i$  and  $P_i$  effects for dichlorobenzenes obtained by using the  $I$  values measured on the SPB-1 column, those calculated with  $I$  values of trichlorobenzenes taken from literature for the SE-30 column, and those predicted for tetrachlorobenzenes by applying to the retention indices the procedure described in Fig. 4 for  $k'$  values. The first two columns of Table 6 show the  $I$  values used for the calculation, the third and fourth columns the retention indices of tetrachlorobenzenes predicted by using the *ortho*, *meta* and *para* effects and those experimentally measured on the SPB-1 column. The last two columns show the percent error between experimental and predicted  $I$  values and between the retention times predicted and those measured after the injection of the references  $n$ -alkanes.

Table 6

Prediction of the  $I$  and  $t_R$  values of tetrachlorobenzenes by using the  $I$  values of mono- and dichlorobenzenes experimentally measured on an SPB-1 column and those of trichlorobenzenes taken from the literature (Ref. [24]) for an SE-30 column (temperature 140°C): the last two columns of the table show the percent error for the  $I$  and  $t_R$  values

Compound	$I_{\text{exp}}$	$I_{\text{lit}}$	$I_{\text{pred}}$	$I_{\text{exp}}$	$E$ (%)	
	(SPB-1)	(SE-30)		(SPB-1)	$I$	$t_R$
Chlorobenzene	834					
1,2-Dichlorobenzene	1035					
1,3-Dichlorobenzene	1009					
1,4-Dichlorobenzene	1012					
1,2,3-Trichlorobenzene		1217				
1,2,4-Trichlorobenzene		1183				
1,3,5-Trichlorobenzene		1144				
1,2,3,4-Tetrachlorobenzene			1370	1368	0.15	0.48
1,2,3,5-Tetrachlorobenzene			1331	1327	0.27	1.12
1,2,4,5-Tetrachlorobenzene			1328	1327	0.10	0.45

#### 4. Conclusions

The procedure proposed can permit to predict the retention values of all the chlorobenzene isomers by using a few authentic samples and data taken from literature. The accuracy of the prediction is good enough to allow to identify the compounds or to foresee their retention under different analysis conditions. Further experiments are in progress for applying the same procedure to aromatic compounds containing chlorine atoms and other functional groups on the same ring.

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