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A STUDY OF KOVÁTS RETENTION INDICES OF ALIPHATIC SATURATED ESTERS AND THEIR RELATION TO THE POLARITY OF THE STATIONARY PHASE

J. BERMEJO* and M. D. GUILLEN
Instituto Nacional del Carbón y sus Derivados, C.S.I.C., Ap. 73, 33080 Oviedo (Spain)

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SUMMARY

The validity of the equations that relate Kováts retention indices (I_R) to physico-chemical and structural parameters able to account for the different kinds of solute–stationary phase interactions was corroborated by results obtained for 35 aliphatic saturated esters. The polarity of the stationary phase, as defined by McReynolds, is reflected in the coefficients of the equations, which change linearly with this polarity, making it possible to obtain a new equation for the calculation of the I_R values of aliphatic saturated esters on any stationary phase.

INTRODUCTION

The inability of gas chromatography to provide a sure identification of separated compounds is overcome by using supplementary techniques such as mass spectrometry or Fourier transform IR spectroscopy. The Kováts retention index (I_R) (and other retention parameters), however, is of considerable help in the identification of compounds, even when supplementary techniques are available[1]. Therefore, it is worthwhile searching for equations able to give precise I_R values.

Gas chromatographic retention depends mainly on solute boiling points and solute–stationary phase interactions. Interactive energies between spherical molecules are well known and, depending on their nature, their calculation is carried out with the London, Keson and Debye equations. Solute–stationary phase interactions are much more complex, but their study may be attempted by taking the aforementioned molecular interactions as a basis. In the simplest instance, in which related compounds are separated on the same stationary phase, solute–stationary phase interactions should be a function only of the solute properties. Thus, a multi-parameter approach of the general form

$$I_R = m + n\,T_b + p\,P + q\,Q + \ldots \qquad (1)$$

has been proposed, in which P, Q, ... are solute parameters that account for different kinds of solute–stationary phase interactions[2].

When the solutes are hydrocarbons, equations obtained by least-squares regression analysis of I_R on several stationary phases, together with T_b, and a parameter P related to the electronic polarizability (α), give I_R values for all components of a family of compounds with a standard deviation close to the experimental error[2–4].

TABLE I

VALUES OF PARAMETERS USED FOR CALCULATING I_R

*Compound**	T_b^{16} (°C)	R_M (ml/mol)	V_M (ml/mol)	V_W (ml/mol)	n_D^{16}	ε^{17}	μ^{18} (D)
11	31.50	13.03	61.64	32.30	1.3433	8.50	–
21	54.50	17.82	80.80	42.53	1.3598	–	1.96
12	57.00	17.49	79.40	42.52	1.3593	6.79	–
I31	68.20	22.71	100.96	52.75	1.3678	–	–
22	77.06	22.26	97.88	52.75	1.3723	6.09	1.83
13	79.85	22.18	96.31	52.75	1.3775	5.50	1.70
31	81.30	22.42	97.28	52.76	1.3779	7.70	1.91
I32	90.00	26.96	117.15	62.97	1.3773	–	1.86
1I4	92.30	26.81	114.67	62.97	1.3840	–	–
S41	97.00	27.15	115.45	62.98	1.3865	–	–
T42	97.50	31.44	134.06	73.19	1.3853	–	1.93
I41	98.40	27.07	115.35	62.98	1.3857	6.40	1.89
23	99.10	26.77	114.53	62.98	1.3839	5.63	1.83
32	101.60	26.91	115.04	62.98	1.3842	5.68	1.80
14	102.30	26.81	113.68	62.98	1.3878	5.60	1.71
41	106.80	27.32	114.95	62.99	1.3912	–	–
I33	109.50	31.59	134.13	73.20	1.3872	–	–
S42	112.20	31.51	133.27	73.20	1.3888	–	–
I42	117.20	31.62	133.33	73.20	1.3902	5.29	1.87
33	122.30	31.51	131.86	73.21	1.3935	4.70	1.78
2M2B2	124.25	36.14	148.74	83.42	1.4010	–	–
42	126.50	31.49	131.63	73.21	1.3941	5.01	1.86
I34	130.50	36.23	151.59	83.43	1.3936	–	–
51	132.10	31.75	131.21	73.22	1.3992	–	–
I43	136.80	36.11	149.87	83.43	1.3973	–	–
I52	142.00	36.43	150.16	83.43	1.4003	–	1.82
34	143.00	36.16	149.13	83.44	1.4001	4.30	–
43	145.50	36.16	148.72	83.44	1.4014	–	1.79
52	149.25	36.23	148.69	83.44	1.4023	4.75	1.90
61	155.50	36.37	147.72	83.45	1.4071	–	–
I53	160.70	40.81	165.83	93.66	1.4069	4.20	–
2E1B2	162.50	40.73	164.07	93.66	1.4109	–	–
44	166.60	40.81	165.60	93.67	1.4075	–	–
C62	173.00	38.65	146.63	85.65	1.4401	–	–
I54	178.50	45.42	182.91	103.89	1.4110	4.00	–

* Abbreviations: 11 = methyl formate; 21 = ethyl formate; 12 = methyl acetate; I31 = isopropyl formate; 22 = ethyl acetate; 13 = methyl propionate; 31 = propyl formate; I32 = isopropyl acetate; 1I4 = methyl isobutyrate; S41 = *sec.*-butyl formate; T42 = *tert.*-butyl acetate; I41 = isobutyl formate; 23 = ethyl propionate; 32 = propyl acetate; 14 = methyl butyrate; 41 = butyl formate; I33 = isopropyl propionate; S42 = *sec.*-butyl acetate; I42 = isobutyl acetate; 33 = propyl propionate; 2M2B2 = 2-methyl-2-butyl acetate; 42 = butyl acetate; I34 = isopropyl butyrate; 51 = pentyl formate; I43 = isobutyl propionate; I52 = isopentyl acetate; 34 = propyl butyrate; 43 = butyl propionate; 52 = pentyl acetate; 61 = hexyl formate; I53 = isopentyl propionate; 2E1B2 = 2-ethyl-1-butyl acetate; 44 = butyl butyrate; C62 = cyclohexyl acetate; I54 = isopentyl butyrate.

Aliphatic saturated esters are compounds with an average permanent dipole moment (1.8 D) high enough to induce inductive interactions with any stationary phase and dipole–dipole interactions with high-polarity stationary phases; therefore, these compounds are appropriate for testing the general validity of the proposed approach. On the other hand, from the numerous chromatographic studies carried out with esters, useful correlations between I_R and solute properties have only been found for homologous series[5–14].

EXPERIMENTAL

Retention indices at 120°C were taken from the literature[15]. Boiling points (T_b), densities, refractive indices at 20°C (n_D), dielectric constants (ε) and dipole moments (μ) were taken from refs. 16–18. The calculation of the molar refraction (R_M), molar volume (V_M) and Van der Waal's volume (V_W) has been described in a previous paper[19]. Table I gives the values of T_b, R_M, V_M, V_W, n_D, ε and μ used in this work.

The polarities of the stationary phases (P_M) were taken from ref. 20 and are the sum of the ΔI_R values of benzene, butanol, 2-pentanone, nitropropane and pyridine.

Regression coefficients and statistics were calculated by a multiple regression linear program in an HP 1000 computer.

RESULTS AND DISCUSSION

As expected, acceptable correlations between I_R and T_b are found only for I_R values on low-polarity stationary phases[21]. The statistics worsen as the polarity increases (Table II).

The addition of a second parameter, related to α, in order to correct deviations due to dispersive interactions, provides by least-squares regression the equations in Table III, which show that the molar refraction, the Van der Waal's volume and the molar volume are parameters with a similar capacity for accounting for dispersive interactions[2,19]. The stastistics have improved but not enough to reach deviations close to experimental error as happened with hydrocarbons. This is due to the existence of inductive and dipole–dipole interactions, the relative importance of which depends on the polarity of the stationary phase. Therefore, new terms able to account for these interactions must be included in equations for I_R.

TABLE II

EQUATIONS $I_R = f(T_b)$ ON STATIONARY PHASES OF DIFFERENT POLARITY

P_M is the polarity on the McReynolds scale, R the correlation coefficient, s the standard deviation and N the number of compounds.

Stationary phase No.	*Stationary phase*	P_M^{20}	*Equation*	R	s	N
1	SE-30	217	$I_R = 265.68 + 4.34T_b$	0.9987	7.9	35
2	Dioctyl phthalate	831	$I_R = 339.78 + 4.24T_b$	0.9970	11.6	35
3	Oronite Niw	1494	$I_R = 442.09 + 4.11T_b$	0.9913	19.32	35
4	Pluronic F88	1931	$I_R = 531.54 + 3.81T_b$	0.9805	27.02	35
5	Carbowax 1000	2587	$I_R = 600.91 + 3.87T_b$	0.9724	32.85	35

TABLE III

EQUATIONS $I_R = f(T_b, \theta)$, WHERE $\theta = R_M$, V_M OR V_W

R is the correlation coefficient, *s* the standard deviation and *N* the number of compounds.

Stationary phase	*Equation*	*R*	*s*	*N*
1	$I_R = 242.74 + 4.44T_b + 340.51(1/R_M)$	0.9987	7.8	35
	$I_R = 238.03 + 4.45T_b + 1893.60(1/V_M)$	0.9987	7.9	35
	$I_R = 235.68 + 4.46T_b + 1073.44(1/V_W)$	0.9987	7.7	35
2	$I_R = 226.04 + 4.72T_b + 1688.90(1/R_M)$	0.9984	8.5	35
	$I_R = 205.33 + 4.75T_b + 9207.44(1/V_M)$	0.9986	7.9	35
	$I_R = 207.44 + 4.78T_b + 4736.19(1/V_W)$	0.9985	8.2	35
3	$I_R = 244.12 + 4.93T_b + 2939.46(1/R_M)$	0.9956	13.7	35
	$I_R = 203.09 + 5.02T_b + 16367.50(1/V_M)$	0.9956	12.2	35
	$I_R = 213.42 + 5.03T_b + 8183.76(1/V_W)$	0.9960	13.2	35
4	$I_R = 248.23 + 4.99T_b + 4206.72(1/R_M)$	0.9906	18.8	35
	$I_R = 189.29 + 5.11T_b + 23438.43(1/V_M)$	0.9929	16.4	35
	$I_R = 207.00 + 5.12T_b + 11615.09(1/V_W)$	0.9913	18.1	35
5	$I_R = 258.89 + 5.30T_b + 5078.48(1/R_M)$	0.9865	22.9	35
	$I_R = 187.17 + 5.44T_b + 28334.25(1/V_M)$	0.9897	20.1	35
	$I_R = 209.50 + 5.45T_b + 14008.17(1/V_W)$	0.9913	18.1	35

The refractive index, n_D, has been related to electrostatic solute–stationary phase interactions[19,22], and some of its functions such as n_D^2 or $D = (n_D^2 - 1)/(n_D^2 + 2)$ have been reported to account for inductive chromatographic effects[2]. Table IV shows the triparameter equations obtained by regressing n_D^2 or D together with the previous parameters. The improved statistics, however, are not satisfactory when I_R values on polar stationary phases are used. For these stationary phases it would also be necessary to add parameters accounting for the dipole–dipole interactions, such as the dielectric constant ε[23] or the permanent dipole moment μ[22,24]. Unfortunately, experimental values of ε and μ are available for only a limited number of esters (see Table I). Equations obtained by regressing I_R on Carbowax 1000 corresponding to two groups of 16 esters, for which ε or μ (in benzene) are available, are shown in Table V. The statistics of the least-squares regression analyses improve as new parameters are included, finally reaching satisfactory values. It is worthwhile comparing the statistics of the two groups because they reveal that the number and kind of compounds influence the resulting equations, so that in order to obtain valid conclusions it is necessary to include in the least-squares regression analyses data for the highest number of compounds.

The contribution of the stationary phase to I_R should be reflected by the polarity, which is its most representative chromatographic property. In fact, from the equations in Table IV obtained by regressing I_R of 35 esters on five stationary phases of different polarity, together with T_b, V_W and D values, one deduces that coefficients m, p and q (eqn. 1) increase linearly with increasing polarity of the stationary phase, whereas n is independent of the stationary phase.

Equations that relate coefficients and polarity on the McReynolds scale P_M are

TABLE IV

EQUATIONS $I_R = f(T_b, \theta, n_D)$, WHERE $\theta = V_M$ OR V_M

R is the correlation coefficient, s the standard deviation, N the number of compounds and $D = (n_D^2 - 1)/(n_D^2 + 2)$.

Stationary phase	*Equation*	*R*	*s*	*N*
1	$I_R = 13.08 + 4.21T_b + 2378.93(1/V_M) + 1047.07D$	0.9989	7.2	35
	$I_R = -137.67 + 4.19T_b + 2193.14(1/V_M) + 208.17n_D^2$	0.9989	7.1	35
	$I_R = 472.82 + 4.26T_b + 2895.46(1/V_M) - 52.51(1/D)$	0.9988	7.4	35
	$I_R = 491.85 + 4.26T_b + 1590.49(1/V_W) - 56.93(1/D)$	0.9989	7.3	35
2	$I_R = -114.78 + 4.42T_b + 9898.12(1/V_M) + 1490.06D$	0.9990	6.7	35
	$I_R = -308.49 + 4.41T_b + 9617.44(1/V_M) + 284.70n_D^2$	0.9990	6.7	35
	$I_R = 590.54 + 4.45T_b + 10852.04(1/V_M) - 86.15(1/D)$	0.9990	6.8	35
	$I_R = 660.46 + 4.44T_b + 5929.30(1/V_W) - 102.24(1/D)$	0.9990	6.6	35
3	$I_R = -503.73 + 4.27T_b + 17892.64(1/V_M) + 3290.07D$	0.9986	7.9	35
	$I_R = -925.74 + 4.26T_b + 17270.84(1/V_M) + 625.44n_D^2$	0.9985	7.9	35
	$I_R = 1083.19 + 4.32T_b + 20128.04(1/V_M) - 196.84(1/D)$	0.9986	7.8	35
	$I_R = 1209.90 + 4.29T_b + 10920.25(1/V_W) - 225.60(1/D)$	0.9987	7.4	35
4	$I_R = -771.45 + 4.09T_b + 25511.50(1/V_M) + 4472.01D$	0.9971	10.4	35
	$I_R = -1329.19 + 4.09T_b + 24654.27(1/V_M) + 841.32n_D^2$	0.9970	10.6	35
	$I_R = 1406.67 + 4.15T_b + 28640.97(1/V_M) - 272.28(1/D)$	0.9973	10.1	35
	$I_R = 1584.47 + 4.11T_b + 15476.19(1/V_W) - 312.31(1/D)$	0.9975	9.7	35
5	$I_R = -958.89 + 4.23T_b + 30807.29(1/V_M) + 5334.63D$	0.9955	13.3	35
	$I_R = -1621.00 + 4.22T_b + 29785.58(1/V_M) + 1001.79n_D^2$	0.9954	13.5	35
	$I_R = 1644.02 + 4.29T_b + 34563.94(1/V_M) - 325.86(1/D)$	0.9958	12.8	35
	$I_R = 1858.59 + 4.24T_b + 18677.88(1/V_W) - 374.17(1/D)$	0.9961	12.4	35

shown in Table VI. The best correlation is given by p, but probably the differences between R values are due to the accuracy of the experimental data.

From eqn. 1 and the equations in Table VI, the following equation is obtained:

$$I_R = 280.64 + 4.27\,T_b - 13.96\,(1/V_W) - 10.93\,(1/D) + [0.6235 + 7.4595\,(1/V_W) - 0.1440\,(1/D)]P_M \tag{2}$$

Eqn. 2 relates I_R to the solute properties and the polarity of the stationary phase, so it should be valid for calculating the I_R of esters on any stationary phase at a given working temperature*. Its validity was tested by comparing calculated and experimental I_R values on three stationary phases. The results are given in Table VII and include calculated I_R values on squalane. Only 11,I31, 2M2B2 and I54 show appreciable differences between the calculated and experimental I_R values on the three stationary phases. There are other discrepancies between the two I_R values which seem to depend on the stationary phase more than on the nature of the esters, but acceptable differences predominate.

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* Except on stationary phases of very high polarity, for which a dipole–dipole interaction parameter should be included in eqn. 2.

TABLE V

EQUATIONS FOR I_R ON CARBOWAX 1000 FOR TWO GROUPS OF ESTERS

R is the correlation coefficient, *s* the standard deviation and *N* the number of compounds.

Ester group	*Equation*	*R*	*s*	*N*
I	$I_R = 639.19 + 3.57T_b$	0.9956	12.6	16
	$I_R = 455.79 + 4.32T_b + 11475.49(1/V_M)$	0.9981	8.3	16
	$I_R = 1659.27 + 4.01T_b + 27569.25(1/V_M) - 307.66(1/D)$	0.9990	6.0	16
	$I_R = 1549.46 + 4.27T_b + 26400.02(1/V_M) - 276.61(1/D) - 218.36(1/\varepsilon)$	0.9992	5.3	16
II	$I_R = 614.18 + 3.72T_b$	0.9753	21.8	16
	$I_R = 95.98 + 5.71T_b + 36036.02(1/V_M)$	0.9976	6.9	16
	$I_R = 1184.23 + 4.96T_b + 40808.77(1/V_M) - 246.32(1/D)$	0.9990	4.5	16
	$I_R = 1408.80 + 4.82T_b + 42505.97(1/V_M) - 307.20(1/D) + 10.31\mu^2$	0.9992	3.9	16

The elution order obtained on squalane agrees with that of the boiling points, as usual on non-polar or low-polarity phases[15]. As the polarity of the stationary phase increases, changes in the elution order of some of the branched esters occur. These changes are predicted by eqn. 2, with slight exceptions such as 2M2B2 and I53.

In general, I_R values calculated by eqn. 2 are satisfactory, and the alterations that occur in the elution order are also predicted. Some discrepancies might be due to the inaccuracy of the available experimental data. For example, the n_D value of the 2M2B2 (Table I) seems to be high, taking into account that the branched-chain esters have n_D values smaller than those of their isomeric homologues.

TABLE VI

VARIATION OF THE COEFFICIENTS OF THE EQUATION $I_R = f(T_b, V_W, D)$ WITH THE POLARITY OF THE STATIONARY PHASE

R is the correlation coefficient.

Coefficient	*Equation*	*R*
m	$m = 280.64 + 0.6235\ P_M$	0.9867
n	n = constant = 4.27	
p	$p = -13.96 + 7.4595\ P_M$	0.9957
q	$q = -10.93 - 0.1440\ P_M$	0.9886

CONCLUSIONS

I_R values of aliphatic saturated esters on a given stationary phase and at a given temperature can be obtained from equations in which, in addition to the solute boiling point, solute parameters accounting for dispersive, inductive and dipole–dipole solute–stationary phase interactions are included.

Equations obtained by least-squares regression analyses for I_R for a group of

TABLE VII

EXPERIMENTAL AND PREDICTED I_R VALUES AT 120°C

Stationary phases: 6 = squalane ($P_M = 0$); 7 = diisodecyl phthalate ($P_M = 767$); 8 = Pluronic P65 ($P_M = 1581$); 9 = bis(2-ethoxyethyl) phthalate ($P_M = 1817$).

*Compound**	*Phase 6* *I_R (eqn. 2)*	*Phase 7*			*Phase 8*			*Phase 9*		
		I_R^{15}	I_R (eqn. 2)	ΔI_R	I_R^{15}	I_R (eqn. 2)	ΔI_R	I_R^{15}	I_R (eqn. 2)	ΔI_R
11	363	482	496	−14	627	637	−10	641	678	−37
21	463	577	575	+ 2	708	694	+14	728	729	− 1
12	474	–	586	–	711	704	+ 7	734	738	− 4
I31	523	631	619	+12	744	720	+24	770	750	+20
22	561	659	662	− 3	772	770	+ 2	801	801	0
13	574	679	681	− 2	793	794	− 1	818	827	− 9
31	580	684	688	− 4	802	802	0	828	835	− 7
I32	617	697	706	−10	796	801	− 5	827	829	− 2
1I4	628	725	724	+ 1	825	827	− 2	854	857	− 3
S41	648	740	747	− 7	845	853	− 8	877	884	− 7
T42	650	731	736	− 5	817	826	− 9	848	852	− 4
I41	654	749	752	− 3	859	857	+ 2	887	887	0
23	657	749	753	− 4	854	856	− 2	883	886	− 3
32	667	757	764	− 7	867	867	0	897	897	0
14	671	770	772	− 2	881	879	+ 2	909	910	− 1
41	690	786	795	− 9	906	906	0	932	938	− 6
I33	702	780	789	− 9	868	882	−14	905	909	− 4
S42	713	792	802	−10	890	897	− 7	924	925	− 1
I42	735	817	825	− 8	914	922	− 8	948	950	− 2
33	757	846	851	− 5	947	951	− 3	980	980	0
2M2B2	766	847	858	−11	931	956	−25	961	984	−23
42	775	860	870	−10	967	970	− 3	998	999	− 1
I34	792	875	877	− 2	957	966	− 9	990	993	− 3
51	799	892	899	+ 7	1010	1005	+ 5	1043	1036	+ 7
I43	819	909	908	+ 1	999	1001	− 2	1036	1029	+ 7
I52	842	925	933	− 8	1030	1030	0	1067	1059	+ 8
34	846	940	937	+ 3	1037	1034	+ 3	1072	1062	+10
43	857	951	949	+ 2	1051	1048	+ 3	1087	1076	+11
52	873	964	966	− 2	1074	1066	+ 8	1110	1094	+16
61	900	997	998	− 1	1120	1103	+17	1147	1133	+14
I53	922	1017	1013	+ 4	1111	1109	+ 2	1150	1137	+13
2E1B2	930	1025	1025	0	1127	1125	+ 2	1164	1154	+10
44	947	1043	1039	+ 4	1139	1135	+ 4	1176	1163	+13
C62	978	1103	1104	− 1	1239	1238	+ 1	1271	1276	− 5
I54	999	1103	1087	+16	1197	1181	+16	1236	1208	+28

* Abbreviations as in Table I.

esters depend on the number and kind of compounds included, so the general validity of the equations has to be ensured by regressing data of the highest number of compounds.

These results confirm that some properties or structural parameters, related to α, account for the dispersive interactions; n_D^2 or its functions account for the inductive interactions and ε or μ reflect the dipole–dipole interactions.

Coefficients of the equations $I_R = f(T_b, \theta, n_D)$, where θ is V_M or V_W, increase linearly with increasing polarity of the stationary phase, except the coefficient of the boiling point, which is independent of P_M, so that it is possible to obtain a general equation including the polarity of the stationary phase, which allows us to calculate I_R for all aliphatic saturated esters on stationary phases of polarity between 0 and 2000 on the McReynolds scale.

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