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CORRELATION OF TWO CRITERIA OF POLARITY FOR STATIONARY PHASES IN GAS–LIQUID CHROMATOGRAPHY

MICHAL ROTH and JOSEF NOVÁK*
Institute of Analytical Chemistry, Czechoslovak Academy of Sciences, 61142 Brno (Czechoslovakia)

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SUMMARY

Linear relationships between the partial molar excess Gibbs function of a solute methylene group, $\Delta\bar{G}^{E}(CH_2)$, and the average McReynolds constant, ΔI, and between $\Delta\bar{G}^{E}(CH_2)$ and the individual McReynolds constants were determined for a set of 55 liquid stationary phases. All these relationships were identical at the given level of statistical significance. An analysis of the relationships indicates that $\Delta\bar{G}^{E}(CH_2)$ and ΔI are equivalent criteria of polarity for liquid stationary phases and that polarity can adequately be characterized by a single criterion.

INTRODUCTION

McReynolds[1] showed that the selectivity and/or polarity of a stationary phase in gas–liquid chromatography (GLC) can be characterized by differential Kováts' retention indices, ΔI, measured for several deliberately chosen solutes on the given stationary phase and on squalane as a non-polar reference; he evaluated 226 stationary phases in this way. Since then, several algebraic methods have been applied to his set of data in an attempt to systematize the variations in the ΔI values and establish a standard set of stationary phases for GLC. For instance, the Euclidian distance between a given stationary phase and squalane was calculated[2,3] and "principal component" analysis[4,5] as well as factor analysis[6] were applied to the published ΔI data. It was found[7] that a substantial part of the variations in the ΔI values could be attributed to a single factor called "polarity". However, the termodynamic meaning of this factor is somewhat vague[4].

In the initial McReynolds paper[1], stationary phases were grouped according to increasing polarity, which was arbitrarily defined as the arithmetic mean of the ΔI values determined for benzene, 1-butanol, 2-pentanone, 1-nitropropane and pyridine. In this work, the McReynolds constants for 55 GLC stationary phases are correlated with the corresponding values of the partial excess Gibbs function of one mole of solute methylene, $\Delta\bar{G}^{E}(CH_2)$. The latter quantity is a measure of the deviation of the solution of methylene in a given solvent from an ideal solution and can therefore be considered as a thermodynamically defined criterion of polarity for liquid stationary phases[8–15].

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THEORETICAL

McReynolds constants, ΔI_i

Let us consider a monofunctional solute i of the type $(CH_3)_M(CH_2)_NX$ where X is a functional group and N is the only variable in a given homologous series. Provided that the standard molar Gibbs function of sorption for solute i, $\Delta G^0_{sp}(i)$, comprises the sum of the standard Gibbs function contributions corresponding to the individual groups of the solute[16], *i.e.*

$$\Delta G^0_{sp}(i) = M\Delta G^0_{sp}(CH_3) + N\Delta G^0_{sp}(CH_2) + \Delta G^0_{sp}(X) \tag{1}$$

and that $\Delta G^0_{sp}(CH_3) \approx \Delta G^0_{sp}(CH_2)$, the Kováts' retention index of solute i on a given stationary phase, I_i, can be expressed as[17]

$$I_i = 100[n_i + \Delta G^0_{sp}(X)/\Delta G^0_{sp}(CH_2)] \tag{2}$$

where n_i is the number of carbon atoms in the solute molecule. The difference between the retention indices of solute i on stationary phase y and on squalane (sq) is then given by:

$$\Delta I_i = 100[\Delta G^0_{sp}(X)/\Delta G^0_{sp}(CH_2)]_y - 100[\Delta G^0_{sp}(X)/\Delta G^0_{sp}(CH_2)]_{sq} \tag{3}$$

The retention of solute i on squalane is due to dispersive solute–solvent intermolecular interactions. If the functional group of the solute has a sufficiently large dipole moment, induction forces may also play a rôle, but, owing to the relatively low polarizabilities of C–C and C–H (aliphatic) bonds[18], the contribution of such forces is unimportant. However, with other stationary phases (y), orientation, induction and hydrogen-bonding interactions may appreciably contribute to the retention of solute i. The value of the ratio $[\Delta G^0_{sp}(X)/\Delta G^0_{sp}(CH_2)]_y$ in eqn. (3) will increase with increasing significance of these interactions. Hence, the value of ΔI_i is a measure of the extent to which non-dispersive intermolecular forces contribute to the retention of solute i on stationary phase y, and the arithmetic mean of ΔI_i values measured for several solutes, ΔI, can be considered as a plausible criterion of polarity for stationary phases.

Partial excess Gibbs function of one mole of solute methylene, $\Delta G^E(CH_2)$

The concept of the additivity of the contributions of individual groups in the solute molecule to the partial molar excess Gibbs function of solute in a solute–stationary phase system was introduced by Pierotti *et al.*[19]. The partial excess Gibbs function of one mole of solute methylene has been proposed[8–12] and employed[8–15] as a criterion of polarity for chromatographic stationary phases. It can formally be written for a given stationary phase and a given homologous series of compounds $(CH_3)_M(CH_2)_NX$ at a given temperature as

$$\Delta G^E(CH_2) = -RT\, d\ln(V^0_g P^0)/dN \tag{4}$$

and for two consecutive members of the series, $i_N = (CH_3)_M(CH_2)_NX$ and $i_{N-1} = (CH_3)_M(CH_2)_{N-1}X$, we obtain:

$$\Delta G^{E}(CH_2) = RT \ln [V_g^0 P^0(i_N)/V_g^0 P^0(i_{N+1})] \tag{5}$$

The reluctance of a stationary phase (solvent) to mix with a solute is reflected in the excess enthalpy of the solute–solvent system, ΔH^E. This reluctance is due to different types and intensities of solute–solute and solvent–solvent intermolecular interactions. Since it is the change in the system's potential energy associated with the solution formation that contributes most to the respective enthalpy of mixing, ΔH^E can be expressed according to lattice theory[20] as

$$\Delta H^E = zN_A \Delta w = zN_A \left[\tfrac{1}{2}(w_{11} + w_{22}) - w_{12}\right] \tag{6}$$

where z is the lattice coordination number, N_A is the Avogadro constant and w_{11}, w_{22} and w_{12} are the pairwise potential energies of the solvent–solvent, solute–solute and solvent–solute intermolecular interactions, respectively.

Let us consider the mixing of a given solvent with a paraffinic solute. The solute molecules interact with each other only by means of dispersion forces, whereas the solvent–solvent interactions may involve also interactions by induction and orientation forces and/or by hydrogen bonding, according to the constitution of the solvent molecule. Random mixing of a paraffinic solute with a large excess of solvent to produce an infinitely dilute solution results in the cancellation of all solute–solute interactions and a certain proportion of the solvent–solvent interactions. This destabilization of the system is compensated for by dispersion and, if applicable, inductive solute–solvent interactions. If the solvent is also a paraffin, this compensation is fairly complete, *i.e.*, $(w_{11} + w_{22})/2 \approx w_{12}$. In such a case, for the partial molar enthalpies of two consecutive paraffinic solute homologues, p_N and p_{N+1}, we can write $\Delta H^E(p_N) \approx \Delta H^E(p_{N+1})$, *i.e.*, $\Delta H^E(CH_2) \approx 0$. With non-paraffinic solvents, orientation and/or specific interactions contribute to the value of w_{11}, the importance of these contributions increasing with increasing proportion of groups with large dipole moments in the solvent molecule. The decrease in the intensity of these polar interactions on mixing the solvent with a paraffinic solute is only partially compensated by dispersive and inductive solute–solvent interactions, *i.e.*, $(w_{11} + w_{12})/2 > w_{12}$, and the system will display a positive excess enthalpy. Within a homologous series of solutes $(CH_3)_M(CH_2)_NX$, the partial molar excess enthalpy of a solute in the solute–solvent system will increase with increasing paraffinic portion that the solute molecule introduces into the system, consequently, $\Delta H^E(CH_2) > 0$.

Let us suppose that there is a linear relationship between ΔH^E and ΔS^E (ref. 21) and, consequently, a direct proportionality between $\Delta H^E(CH_2)$ and $\Delta S^E(CH_2)$ for a given solvent and a given homologous series of solutes $(CH_3)_M(CH_2)_NX$ at a given temperature. Then there is also a direct proportionality between $\Delta H^E(CH_2)$ and $\Delta G^E(CH_2)$, and the latter quantity actually characterizes the ability of the stationary phase to interact with solutes of the type $(CH_3)_M(CH_2)_NX$ by means of intermolecular forces other than dispersive ones. Hence, the average partial excess Gibbs function per mole of solute methylene, $\Delta \overline{G}^E(CH_2)$, determined from data measured for several different types of solutes, on a given stationary phase, can be looked upon as a representative measure of the polarity of the stationary phase[8–15]. This is illustrated in Fig. 1 by the dependences of $-RT \ln (V_g^0 P^0)$ on N for several typical stationary phases and straight-chain alkanols as solutes. In view of the above concepts, it is possible to expect a meaningful correlation between $\Delta \overline{G}^E(CH_2)$ and ΔI.

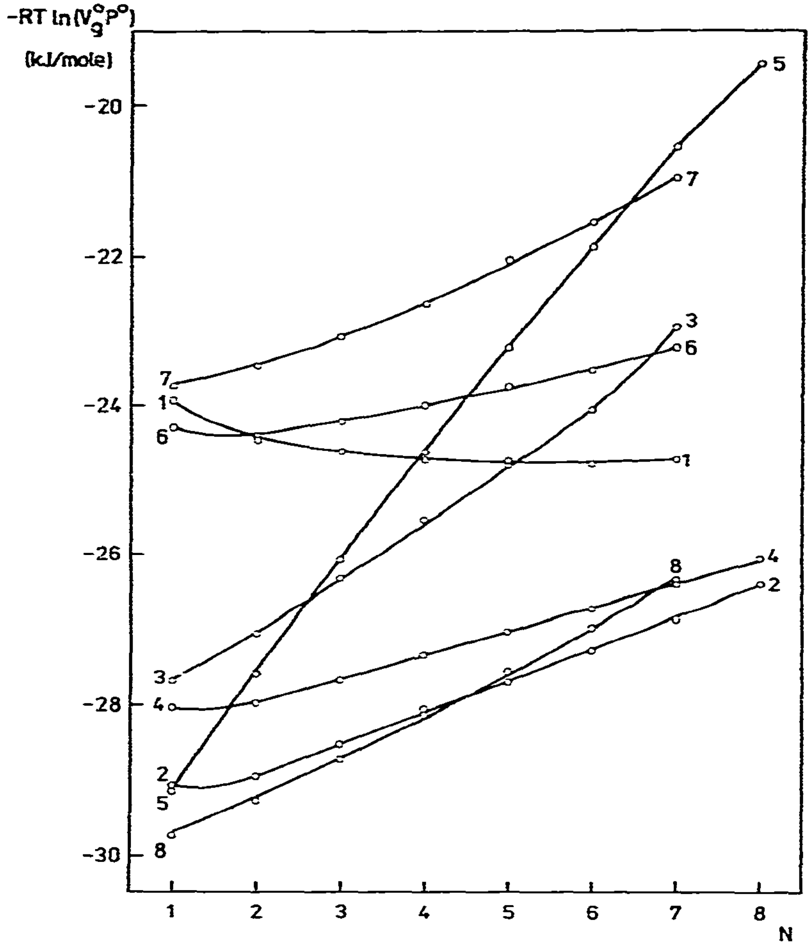

Fig. 1. Plots of $-RT \ln (V_g^0 P^0)$ *versus* methylene number, N for $CH_3(CH_2)_NOH$ alcohols on different stationary phases at 120°C. Phases: 1 = Apiezon L; 2 = Carbowax 20M; 3 = diethylene glycol succinate; 4 = Triton X-305; 5 = diglycerol; 6 = SE-31; 7 = QF-1; 8 = Hyprose SP 80.

RESULTS

The relationships between $\Delta\bar{G}^E(CH_2)$ and the individual ΔI_i values and between $\Delta\bar{G}^E(CH_2)$ and ΔI at 120°C were determined for a set of 55 liquid stationary phases. With all the stationary phases studied, the McReynolds constants and the retention data necessary to calculate the $\Delta\bar{G}^E(CH_2)$ values were taken from the literature. The stationary phases are listed in the legend to Fig. 2. Each $\Delta\bar{G}^E(CH_2)$ value is an arithmetic mean of the $\Delta G^E(CH_2)$ values determined for a given stationary phase from the specific retention volumes[22] and saturation vapour pressures[23] of pairs of homologous straight-chain 1-alkanols, 1-alkanals, 2-alkanones, *n*-alkyl acetates, symmetrical di-*n*-alkyl ethers and alkanes by

$$\Delta G^E(CH_2) = \frac{1}{k} RT \ln \frac{V_g^0 P^0(i_N)}{V_g^0 P^0(i_{N+k})} \tag{7}$$

TABLE I

SOLUTES USED TO DETERMINE $\Delta \bar{G}^E(CH_2)$

Solutes	*k*	*Homologue i_N*	*Homologue i_{N+k}*
1-Alkanols	1	1-Pentanol	1-Hexanol
1-Alkanals	2	1-Pentanal	1-Heptanal
2-Alkanones	1	2-Hexanone	2-Heptanone
n-Alkyl acetates	1	*n*-Pentyl acetate	*n*-Hexyl acetate
Di-*n*-alkyl ethers	2	Di-*n*-butyl ether	Di-*n*-pentyl ether
n-Alkanes	2	*n*-Octane	*n*-Decane

where k is either 1 or 2. The solutes are specified in Table I. Let us recall[12] that the value of $\Delta G^E(CH_2)$ is only slightly dependent on the type of solutes employed. The ΔI_i values (i = benzene, 1-butanol, 2-pentanone, pyridine, 1-nitropropane, 2-methyl-2-pentanol and 2-octyne) were taken from the initial McReynolds paper[1]. The parameters of the linear correlations of $\Delta \bar{G}^E(CH_2)$ with the individual ΔI_i values are summarized in Table II. In Fig. 2, the $\Delta \bar{G}^E(CH_2)$ values are plotted against the corresponding values of ΔI, the latter being the arithmetic means of the individual ΔI_i values exclusive of those of 2-methyl-2-pentanol and 2-octyne. Linear regression of the data in Fig. 2 yielded the relation

$$\Delta \bar{G}^E(CH_2) = 1.064\, \Delta I - 18.11$$

the respective correlation coefficient being 0.8591. A comparison of this correlation coefficient and those shown in Table II with the tabulated critical values[24] indicates that there is, with a probability greater than 99%, a linear relationship between $\Delta \bar{G}^E(CH_2)$ and ΔI_i as well as between $\Delta \bar{G}^E(CH_2)$ and ΔI within the set of stationary phases studied. Further, a statistical evaluation[25] of the parameters of the regression relations shows that with all the relations the intercepts are, with a probability greater than 99%, statistically insignificant. Hence, the dependence of $\Delta \bar{G}^E(CH_2)$ on ΔI_i as well as the dependence of $\Delta \bar{G}^E(CH_2)$ on ΔI can equally well be represented by a direct proportionality $\Delta \bar{G}^E(CH_2) = q\, \Delta I_i$ and/or $\Delta \bar{G}^E(CH_2) = q\, \Delta I$, the value of q being significantly different from unity only with i = benzene, 2-pentanone and 2-octyne.

TABLE II

PARAMETERS OF THE CORRELATION OF $\Delta \bar{G}^E(CH_2)$ WITH ΔI_i

Solute	*Slope*	*Intercept*	*Correlation coefficient*
Benzene	1.506	16.42	0.8166
1-Butanol	0.886	− 8.37	0.8268
2-Pentanone	1.272	−22.92	0.8798
1-Nitropropane	0.885	−29.84	0.8416
Pyridine	0.900	0.38	0.8725
2-Methyl-2-pentanol	1.165	− 5.07	0.8317
2-Octyne	1.977	51.17	0.7167

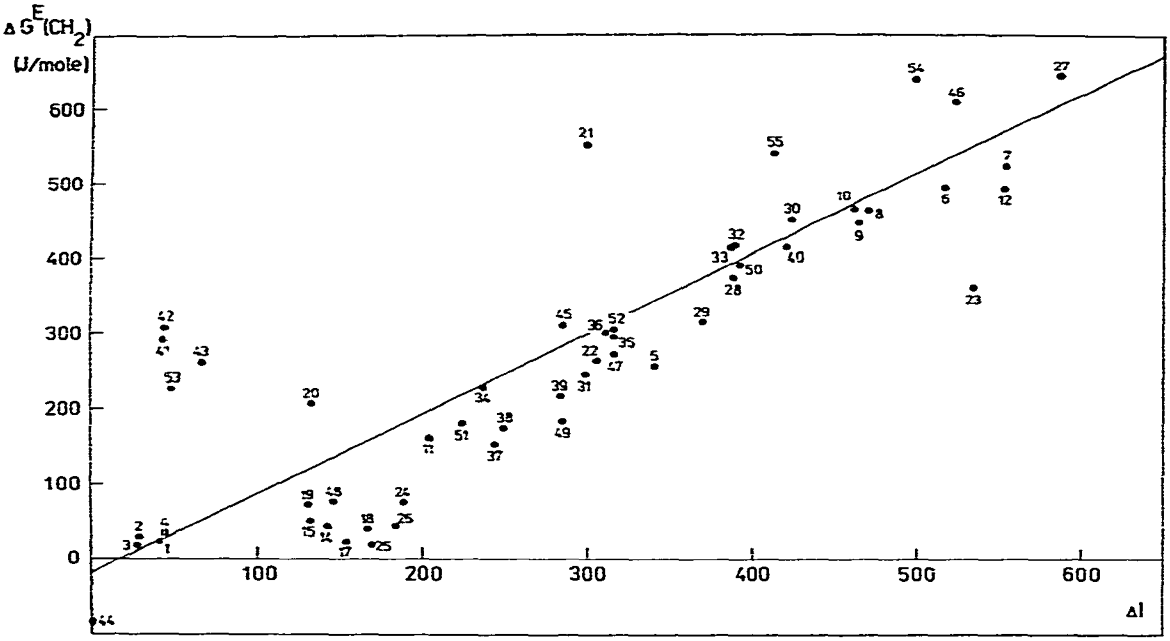

Fig. 2. Correlation of $\Delta\bar{G}^E(CH_2)$ with ΔI. Phases: 1 = Apiezon J; 2 = Apiezon L; 3 = Apiezon M; 4 = Apiezon N; 5 = bis(2-ethoxyethyl) phthalate; 6 = Carbowax 1000; 7 = Carbowax 1540; 8 = Carbowax 4000; 9 = Carbowax 6000; 10 = Carbowax 20M; 11 = Castorwax; 12 = diethylene glycol adipate; 13 = diethylene glycol succinate; 14 = di-2-ethylhexyl adipate; 15 = di-2-ethylhexyl sebacate; 16 = diglycerol; 17 = diisodecyl phthalate; 18 = dioctyl phthalate; 19 = dioctyl sebacate; 20 = Dow Corning 550 Fluid; 21 = Dow Corning FS 1265 Fluid (QF-1); 22 = Ethofat 60-25; 23 = ethylene glycol adipate; 24 = Flexol 8N8; 25 = Hallcomid M 18; 26 = Hallcomid M 18 OL; 27 = Hyprose SP 80; 28 = Igepal CO 880; 29 = neopentyl glycol adipate; 30 = neopentyl glycol succinate; 31 = Oronite NIW; 32 = Pluronic F 68; 33 = Pluronic F 88; 34 = Pluronic L 81; 35 = Pluronic P 65; 36 = Pluronic P 85; 37 = poly(phenyl ether), five rings; 38 = poly(phenyl ether), six rings; 39 = Polytergent J 300; 40 = Quadrol; 41 = SE-30; 42 = SE-31; 43 = SE-52; 44 = squalane; 45 = sucrose acetate isobutyrate; 46 = sucrose octaacetate; 47 = Tergitol NPX; 48 = TMP tripelargonate; 49 = tricresyl phosphate; 50 = Triton X-305; 51 = Ucon LB-1715; 52 = Ucon 50 HB-2000; 53 = Versilube F-50; 54 = XF-1150; 55 = Zonyl E 7. Diethylene glycol succinate (13) and diglycerol (16) are not shown on the plot; the coordinates of the respective points are ΔI = 708.6, $\Delta\bar{G}^E(CH_2)$ = 707.6 J/mol (13) and ΔI = 657.4, $\Delta\bar{G}^E(CH_2)$ = 1071.8 J/mol (16).

DISCUSSION

The data in Fig. 2 show that the stationary phases can be arranged into the following series according to increasing $\Delta\bar{G}^E(CH_2)$ values: squalane, Apiezons, amides, esters, polyethers, substances containing highly-acidic hydrogen. However, this is merely a rough classification. The position of a stationary phase of a given chemical type in the $\Delta\bar{G}^E(CH_2)$ *versus* ΔI plot depends appreciably on its molecular constitution, the most important factors in this respect being the content of polar groups relative to that of non-polar ones and the steric accessibility of the polar groups. For instance, the significantly larger $\Delta\bar{G}^E(CH_2)$ value of sucrose octaacetate (610 J/mol) than that of sucrose diacetate hexaisobutyrate (312 J/mol) is apparently due to the greater steric hindrance of the ether and carbonyl oxygens by the isopropyl groups in the latter compared with that by the methyl groups in the former. Hence, the $\Delta\bar{H}^E(CH_2)$ of sucrose octaacetate is larger than that of sucrose diacetate hexaisobutyrate. In addition, as the diacetate hexaisobutyrate is more bulky than the octaacetate, the entropic component[21] of $\Delta\bar{G}^E(CH_2)$, $T\Delta\bar{S}^E(CH_2)$, will apparently be larger for the former, thus decreasing the respective $\Delta\bar{G}^E(CH_2)$ value. The rôle of the entropic component of $\bar{G}^E(CH_2)$ is especially important when comparing stationary phases of markedly different molar volumes. For instance, the difference between the $\Delta\bar{G}^E(CH_2)$ values of diglycerol (1071.8 J/mol) and Hyprose SP-80 (646.0 J/mol) is probably only due to the different contributions of $T\Delta\bar{S}^E(CH_2)$. In this context, it should be noted that whereas with $\Delta\bar{G}^E(CH_2)$ the $T\Delta\bar{S}^E(CH_2)$ component will be manifested in full, with ΔI (*cf.*, eqns. 2 and 3) the $T\Delta S_{sp}(X)$ and $T\Delta S_{sp}(CH_2)$ terms may be reduced to some degree in the ratios $\Delta G_{sp}(X)/\Delta G_{sp}(CH_2)$.

With silicone stationary phases the $\Delta\bar{G}^E(CH_2)$ values show marked positive deviations from the correlation line. In particular, the $\Delta\bar{G}^E(CH_2)$ values of non-polar silicone phases are much larger than one would expect on the basis of their McReynolds constants. Since the courses of the dependences of $-RT\ln(V_g^0P^0)$ on N for homologous solutes chromatographed on silicone stationary phases are as regular as those on the other stationary phases investigated (*cf.*, Fig. 1), this anomaly can hardly be interpreted as being due to non-additivity of the ΔG^E values of the individual groups in the solute molecule. A similar anomaly was observed in the retention behaviour of homologous *n*-alkanes chromatographed on silicone stationary phases[26].

CONCLUSIONS

The average McReynolds constant and the partial excess Gibbs function of one mole of methylene group are based on very different concepts and have different thermodynamic meanings. Whereas the first quantity reflects the relative affinity of the stationary phase towards an "average" functional group and a methylene group of solute, the second is a measure of the reluctance of the stationary phase to accommodate a methylene group. In spite of these differences, it can be stated that ΔI and $\Delta\bar{G}^E(CH_2)$ are equivalent criteria of polarity for liquid stationary phases; the coordinates of points lying on the regression line in the $\Delta\bar{G}^E(CH_2)$ *versus* ΔI plot even have (incidentally) the same numerical values.

Strictly speaking, considerations of the polarity of solvents should be based exclusively on the type and intensity of the intermolecular solute–solvent interactions, *i.e.*, the partial excess enthalpy of one mole of methylene group, $\Delta\bar{H}^E(CH_2)$, is a more adequate criterion of polarity. However, the determination of $\Delta\bar{H}^E(CH_2)$ requires much more experimental data compared with $\Delta\bar{G}^E(CH_2)$ and is much more sensitive to errors incidental to the experimental determination of activity coefficients[21]. A necessary condition for $\Delta\bar{G}^E(CH_2)$ to be a representative polarity criterion is the existence of a direct proportionality between the $\Delta G^E(CH_2)$ and $\Delta H^E(CH_2)$ in the solute–solvent system, which is fulfilled if there is a direct proportionality between $\Delta H^E(CH_2)$ and $\Delta S^E(CH_2)$. The fact that this condition is not fulfilled with some systems, and the difference in the weights of the entropic effects with $\Delta\bar{G}^E(CH_2)$ and with ΔI, are the most likely reasons for the scattering of the points about the regression line in Fig. 2. The equivalence of $\Delta\bar{G}^E(CH_2)$ and ΔI as polarity criteria on the one hand and statistically insignificant differences between the correlation of $\Delta\bar{G}^E(CH_2)$

versus ΔI and that of $\Delta\bar{G}^E(CH_2)$ *versus* ΔI_i on the other indicate that the polarity of a stationary phase can adequately be characterized by a single criterion.

LIST OF SYMBOLS

$\Delta G^0_{sp}(i)$	Standard molar Gibbs function of sorption of solute i
$\Delta G^0_{sp}(X)$	Increment of functional group X to $\Delta G^0_{sp}(i)$
ΔG^E	Excess Gibbs function of the solute–solvent system*
$\Delta G^E(CH_2)$	Partial excess Gibbs function of one mole of solute methylene group
$\Delta\bar{G}^E(CH_2)$	Average of $\Delta G^E(CH_2)$ values of solutes listed in Table I
ΔH^E	Excess enthalpy of the solute–solvent system
$\Delta H^E(CH_2)$	Partial excess enthalpy of one mole of solute methylene group
I_i	Kováts' retention index of solute i on a given stationary phase, y
ΔI_i	Difference $I_i^y - I_i^{\text{squalane}}$ (McReynolds constant)
ΔI	Average value of ΔI_i; $\Delta I = \frac{1}{5} \sum_i \Delta I_i$, where i = benzene, 1-butanol, 2-pentanone, 1-nitropropane and pyridine
M	Number of methyl groups in the solute molecule
N	Number of methylene groups in the solute molecule
N_A	Avogadro number
n	Number of carbon atoms in the solute molecule
P^0	Saturation vapour pressure of solute
ΔS^E	Excess entropy of the solute–solvent system
$\Delta S^E(CH_2)$	Partial excess entropy of one mole of solute methylene group
V_g^0	Specific retention volume of solute
w_{ij}	Pairwise potential energy of the interaction of molecules of compounds i and j
Δw	$\frac{1}{2}(w_{11} + w_{22}) - w_{12}$, where subscripts 1 and 2 refer to solvent and solute, respectively
z	Lattice coordination number

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* All excess quantities refer to infinite dilution of solute.

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