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Journal of Chromatography A, 893 (2000) 339–346

JOURNAL OF
CHROMATOGRAPHY A

www.elsevier.com/locate/chroma

Calculation of Abraham solute descriptors from McReynolds gas chromatographic retention data

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Received 12 April 2000; received in revised form 5 July 2000; accepted 6 July 2000

Abstract

Quantitative descriptors of solubility properties are useful in the investigation of a wide variety of chemical and biological phenomena. Several solutes which may be useful in such studies are not suitable because these values have not been previously determined experimentally. Several solute descriptors used in the linear solvation energy relationship developed by Abraham and co-workers have been calculated either algebraically or by multiple linear regression analysis. Values for those descriptors which have been calculated are reported and the methods of calculation of these descriptors are also discussed. It is shown that both methods of determination of missing solute descriptor values agree statistically with each other and that the values reported for the calculated descriptors correlate well with data previously reported for similar homologs. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Solute descriptors; Linear solvation energy relationships; Multiple linear regression analysis; Regression analysis

1. Introduction

Because solubility phenomena play an important role in numerous chemical processes, several models describing solute/solvent interactions have been reported [1–6]. Of particular interest are the linear solvation energy relationships (LSERs) of Kamlet, Abraham, and Taft [3], which describe the relative contributions of several intermolecular interactions to the solvation process. The most current version of this LSER, developed by Abraham and co-workers, consists of several additive terms each of which consists of a solvent and a solute descriptor related to

specific intermolecular interactions [4,5]. This LSER is given as follows:

$$\log SP = c_1 + r_1 R_2 + s_1 \pi_2^H + a_1 \Sigma \alpha_2^H + b_1 \Sigma \beta_2^H + l_1 \log L^{16} \quad (1)$$

In this equation $\log SP$ refers to the base ten logarithm of any solubility property; customarily the specific retention volume, V_g , or the thermodynamic partition coefficient, K , is used. The coefficients with subscript 1 characterize the solvent under investigation; the corresponding terms with subscript 2 describe the various intermolecular interactions of the solute as they contribute to the solvation process. The $r_1 R_2$ term is an excess molar refractivity term; this term is influenced by the electron density of π -bonds and lone electron pairs. The $s_1 \pi_2^H$ term is a

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dipolarity/polarizability term, whereas the $l_1 \log L^{16}$ term corresponds to dispersion and cavity formation interactions. The other two terms, $a_1 \Sigma \alpha_2^H$ and $b_1 \Sigma \alpha_2^H$, contain complementary interactions. $\Sigma \alpha_2^H$ describes the hydrogen-bond donor acidity of the solute; thus, a_1 gives the relative contribution of H-bond acceptor basicity of the solvent. Likewise, $\Sigma \beta_2^H$ refers to the H-bond acceptor basicity of the solute; b_1 corresponds to the H-bond donor acidity of the solvent.

The terms which characterize the solute (those with subscript 2) are available for a vast number of compounds [7]. The values for these descriptors have been utilized with numerous gas chromatographic retention data sets [4,8–14] to calculate, by multiple linear regression analysis (MLRA), the coefficients with subscript 1, which characterize the solvent of interest. The solute descriptors are typically determined by solvatochromic methods; in other words, interactions of these solutes with compounds which result in changes in the wave-length of absorption are observed. These changes must be correlatable to the specific descriptor being determined. Unfortunately, several solutes are not amenable to determination of one or more solute descriptors by these methods. Fortunately, however, a significant amount of retention data for many of these solutes exists in the literature, namely, the McReynolds gas chromatographic retention data set [8]. This data set contains retention data for approximately 200–250 solutes on 77 stationary phases. With this data, back calculation of several of these solute descriptors is possible.

Below, the results of back calculation of several solute descriptors are given as well as a description of the mathematical methods which were utilized to determine these values. Additionally, several of these calculated values are compared with solute descriptors for compounds of homologous series, which have been reported previously [7].

2. Methodology

A total of 83 solutes for which at least one solute descriptor needed to be calculated were contained in the McReynolds data set. These solutes are listed in Table 1 along with any solute descriptor values

which are already known. For 53 of these solutes, only the $\Sigma \beta_2^H$ term needed to be calculated. Initial attempts to calculate this parameter included solving for $\Sigma \beta_2^H$ algebraically as well as performing linear regression where the $\Sigma \beta_2^H$ term was the only unknown coefficient. Because only 20 stationary phases from the McReynolds data set had a statistically significant b_1 coefficient and because several of the values were only marginally significant, back calculation of the $\Sigma \beta_2^H$ term was determined to be impractical.

For the remaining 30 solutes, several were missing the $\Sigma \beta_2^H$ term; this term was not calculated for these solutes. Lack of values for this descriptor does not pose significant problems when evaluating new phases (solvents) as a vast majority of solvents that are characterized by LSER have insignificant $b_1 \Sigma \beta_2^H$ terms and this term is subsequently eliminated.

For these 30 solutes determination of the solute descriptors was performed by either one or two methods depending on whether more than one solute descriptor was missing or just one value needed to be determined. If at least two descriptors needed to be determined, only MLRA was performed and the coefficients determined corresponded to the solute descriptors that were missing. With this approach, the regression constant along with any terms for which a solute descriptor was known had to be subtracted from the $\log V_g$ in order to perform the regression. This resulting term was the dependent variable and the coefficients determined by MLRA corresponded to the appropriate solute descriptors. A typical calculation might require that $\Sigma \alpha_2^H$ and π_2^H be calculated by MLRA. Upon rearranging the LSER, the relationship would have the following form:

$$\log V_g - (c_1 + r_1 R_2 + l_1 \log L^{16}) = s_1 \pi_2^H + a_1 \Sigma \alpha_2^H \quad (2)$$

Ideally, the regression constant from this MLRA should be zero; in several cases, the MLRA produced a constant which did not differ significantly from zero. Because back calculation of solute descriptors for several solutes produced regression constants that were not statistically close to zero, it was decided to calculate all solute descriptors while forcing the intercept through zero. For these solutes, the descriptor values for both methods of MLRA are reported.

Table 1
Solute for which at least one solute descriptor is unavailable

Solute	R_2	π_2^H	$\Sigma\alpha_2^H$	$\Sigma\beta_2^H$	Log L^{16}
<i>n</i> -Propoxy- <i>s</i> -butoxymethane	0.000	0.40	0.00	N/A	4.037
Hexa-2,4-dienal	0.769	0.90	0.00	N/A	3.800
Ethoxyisopropoxymethane	0.000	0.41	0.00	N/A	3.093
1,1-Dimethoxybutane	0.010	0.47	0.00	N/A	3.313
1,1-Dimethoxypropane	0.030	0.46	0.00	N/A	2.841
Ethoxy- <i>n</i> -propoxymethane	0.000	0.44	0.00	N/A	3.280
But-3-ene-2-ol	0.295	0.43	0.35	N/A	2.206
Diisopropoxymethane	0.000	0.37	0.00	N/A	3.376
Ethylene diacetate	0.169	1.18	0.00	N/A	3.937
1,2-Dimethoxyethane	0.116	0.66	0.00	N/A	2.565
4-Hydroxybutan-2-one	0.340	0.85	0.41	N/A	3.160
1-Hydroxy-2-methylbutan-3-one	0.342	0.81	0.41	N/A	3.573
Butan-2,3-dione, biacetyl	0.220	0.94	0.00	N/A	1.639
1,1-Diethoxyethane, acetal	0.000	0.41	0.00	N/A	3.066
Isopropenyl acetate	0.196	0.68	0.00	N/A	2.611
Dimethoxymethane	0.088	0.52	0.00	N/A	1.894
Diisobutoxymethane	0.000	0.35	0.00	N/A	4.331
1,1-Dimethoxyethane	0.062	0.49	0.00	N/A	2.334
2-Hydroxy-2-methylbutan-3-one	0.234	0.75	0.21	N/A	2.951
Trioxan	0.100	1.03	0.00	N/A	2.650
Di- <i>s</i> -butoxymethane	0.000	0.37	0.00	N/A	4.380
1,1-Diisobutoxyethane	0.000	0.26	0.00	N/A	4.491
Allyl propanoate	0.179	0.67	0.00	N/A	3.241
1,3-Propylene oxide	0.319	0.61	0.00	N/A	2.086
Di- <i>n</i> -propoxymethane	0.000	0.42	0.00	N/A	3.762
3-Hydroxybutan-2-one	0.289	0.78	0.28	N/A	2.771
Methoxyethoxymethane	0.030	0.49	0.00	N/A	2.371
2-Methoxypropan-1-ol	0.240	0.58	0.40	N/A	2.793
2-Methylbut-3-yne-2-ol	0.292	0.47	0.46	N/A	2.209
3-Ethoxypropan-1-ol	0.230	0.57	0.40	N/A	3.426
3-Methoxybutan-1-ol	0.225	0.66	0.35	N/A	3.398
Vinyl butanoate	0.200	0.56	0.00	N/A	3.191
Di- <i>n</i> -butoxymethane	0.000	0.43	0.00	N/A	4.726
Methylene diacetate	0.154	1.18	0.00	N/A	3.419
1,1-Diethoxypropane	0.000	0.38	0.00	N/A	3.498
Methoxyisopropoxymethane	0.000	0.45	0.00	N/A	2.697
Pent-3-ene-1-ol	0.323	0.50	0.35	N/A	3.064
Diethoxymethane	0.015	0.45	0.00	N/A	2.789
Ethoxy- <i>s</i> -butoxymethane	0.000	0.41	0.00	N/A	3.609
2-Ethoxypropan-1-ol	0.207	0.56	0.40	N/A	3.115
4-Methoxy-4-methylpentan-2-ol	0.170	0.65	0.35	N/A	3.963
Pentan-2,3-dione	0.212	0.47	0.00	N/A	2.209
Acetylacetone, pentan-2,4-dione	0.412	0.56	0.00	N/A	2.918
2-Allyloxyethanol	0.332	0.64	0.41	N/A	3.283
1-Propoxypropan-2-ol	0.210	0.57	0.35	N/A	3.495
1-Ethoxypentan-3-ol	0.220	0.60	0.35	N/A	4.102
1-Methoxypropan-2-ol	0.218	0.61	0.35	N/A	2.655
2-Methylpropan-1,2-diol	0.350	0.60	0.56	N/A	3.190
3-Methylbut-3-ene-2-one	0.297	0.68	0.00	N/A	2.691
<i>dl</i> -Butan-2,3-diol	0.341	0.62	0.55	N/A	3.250
Butan-1,2-diol	0.361	0.63	0.63	N/A	3.525
<i>meso</i> -Butan-2,3-diol	0.365	0.65	0.55	N/A	3.291
Butan-1,3-diol	0.377	0.68	0.64	N/A	3.642
2-Ethylbutanal	0.140	0.62	0.00	0.45	N/A

Table 1. Continued

Solute	R_2	π_2^H	$\Sigma\alpha_2^H$	$\Sigma\beta_2^H$	$\log L^{16}$
Cyclohexyl acetate	0.283	0.69	0.00	N/A	N/A
4-Hydroxy-4-methylpentan-2-one	0.223	0.83	N/A	0.18	3.475
1,1,3-Trimethoxybutane	0.028	0.69	N/A	N/A	3.962
Di(2-ethoxyethyl) ether	0.037	N/A	0.00	N/A	4.592
Cyclopropylcarbinol	0.381	N/A	N/A	N/A	2.675
1,1-Diisopropoxyethane	0.000	N/A	0.00	N/A	N/A
1,3-Dioxolane	0.298	N/A	0.00	N/A	N/A
Isobutyl vinyl ether	0.112	N/A	0.00	N/A	2.746
<i>n</i> -Butyl vinyl ether	0.144	N/A	0.00	N/A	2.970
Allyl formate	0.250	N/A	0.00	N/A	2.256
2-Methyl-2,4-pentandiol	0.242	N/A	N/A	N/A	N/A
2-Methoxyethyl vinyl ether	0.160	N/A	0.00	N/A	2.932
2-Methyl-1,3-dioxolane	0.241	N/A	0.00	N/A	N/A
2-Methylcyclohexanol	0.442	N/A	N/A	N/A	4.110
4,5-Dimethyl-1,3-dioxolane	0.200	N/A	0.00	N/A	N/A
Prop-2-yne-1-ol	0.406	N/A	N/A	0.30	2.050
4-Methyl-1,3-dioxolane	0.240	N/A	0.00	N/A	N/A
2-Ethyl-1-hexyl acrylate	N/A	N/A	N/A	N/A	5.445
Allyl acrylate	N/A	0.72	0.00	N/A	3.160
1,2-Di- <i>n</i> -butoxyethane	N/A	0.51	0.00	N/A	5.176
3-Methoxy-1-butyl acetate	N/A	0.83	N/A	N/A	4.048
3-Methoxy-1-butyl acrylate	N/A	0.83	N/A	N/A	4.048
Ethylene dipropionate	N/A	1.05	N/A	N/A	4.914
Di(2-ethyl-1-butyl) ether	N/A	N/A	N/A	N/A	5.421
1-Propenyl acetate	N/A	0.67	N/A	N/A	2.741
Propylene diacrylate	N/A	1.10	N/A	N/A	4.979
2-Ethyl-1-hexyl vinyl ether	N/A	N/A	N/A	N/A	4.682
Ethylidene diacetate	N/A	N/A	N/A	N/A	N/A
2,2-Dimethylpropan-1,3-diol	0.350	N/A	N/A	N/A	N/A

Algebraic calculation of one descriptor is straightforward; all terms for which both the variable and coefficient are known are subtracted from $\log V_g$ leaving this one term equal to the term for which a solute descriptor is to be determined. Dividing both sides of the equation by the corresponding LSER coefficient results in an expression to calculate the unknown descriptor. As an example, back calculation of π_2^H would utilize the following expression:

$$[\log V_g - (c_1 + r_1 R_2 + l_1 \log L^{16} + a_1 \Sigma \alpha_2^H)] / s_1 = \pi_2^H \quad (3)$$

For three solutes, 2-ethyl-1-hexyl vinyl ether, di(2-ethyl-1-butyl) ether, and ethylidene diacetate, the *p*-value indicated that the $r_1 R_2$ and $a_1 \Sigma \alpha_2^H$ terms were statistically insignificant. Based on the structure of these three solutes, this makes sense chemically;

as a result, these terms were eliminated and the remaining unknown descriptors were calculated. In the cases of 2-ethyl-1-hexyl vinyl ether and di(2-ethyl-1-butyl) ether, elimination of these two terms left only the π_2^H term to calculate; thus an algebraic calculation was performed. When determining the average π_2^H value and the standard deviation from the algebraic calculation, the value on squalane was eliminated by performing the *Q*-test.

3. Results and discussion

Of the 30 solutes for which at least one descriptor was missing (other than $\Sigma \beta_2^H$), back calculation of solute descriptors for two of these solutes was not attempted because no retention data exists in the

McReynold's data set. These two solutes were 2,2-dimethylpropan-1,3-diol and 2-methyl-2,4-pentandiol.

For eight solutes, reliable back calculation of missing solute descriptors was impractical due to the relatively small values for the dependent variable in the regression. Due to the nature of MLRA calculations, it is necessary to have dependent variables which cover a sufficiently large range to permit accurate back calculation of solute descriptors. These eight solutes were 1-propenyl acetate, ethylene dipropanoate, allyl acrylate, propylene diacrylate, 1,2-di-*n*-butoxyethane, 3-methoxy-1-butyl acetate, 3-methoxy-1-butyl acrylate, and 1,1,3-trimethoxybutane. The MLRA leads to results for which the adjusted R^2 is of little value statistically, and the standard error of the relationship is extremely large compared to the dependent variable. In the cases of ethylene dipropanoate and propylene diacrylate, the poor results are compounded by the fact that only 13 phases are available for which retention data exists for the ethylene dipropanoate and 11 phases for the propylene diacrylate.

For 2-ethyl-1-hexyl acrylate, although the values for the dependent variable are large enough to permit back calculation by MLRA, several of the values for the dependent variable are negative and no predictable trend exists between these values and any of the LSER coefficients. Not surprisingly, the adjusted R^2 is extremely low (0.38), and the standard error is significantly larger than desirable (0.43). As a result, values for this solute are not reliable and are not reported.

For 2-methyl-1,3-dioxolane, the values of the dependent variable are statistically large enough to permit analysis by MLRA; however, the adjusted R^2 is only 0.55 and the standard error is 0.20. When the intercept is calculated while performing MLRA, the value is -2.18 , significantly different from zero. If the MLRA is forced through zero, the values of the descriptors change markedly and the adjusted R^2 drops to 0.41.

For the remaining 18 solutes, results of back calculation of solute descriptors are summarized in Table 2. Because MLRA for several solutes exhibit a significant non-zero intercept for the MLRA in which the intercept is calculated, results for both MLRA approaches (calculated intercept and intercept

forced through zero) are reported. In addition, results for any algebraically calculated descriptors are also reported in Table 2.

Several solutes in Table 2 have an adjusted R^2 that is marginally low but still statistically significant. In these cases, the standard error is reasonable (approximately 0.02–0.03); the somewhat lower adjusted R^2 is most likely due to values for the dependent variable which are small but significant. As the relative values for the dependent variable increase, the adjusted R^2 increases correspondingly.

Comparing the results for cyclopropyl carbinol with homologous compounds for which solute descriptors have been reported previously [7], the current back calculation approach can be justified. The straight-chain alcohols, propan-1-ol and butan-1-ol, both have π_2^H values of 0.42. When advancing to the cycloalkyl alcohols, cyclopentanol, cyclohexanol, and cycloheptanol, each of these values is 0.54, the same value as cyclopropyl carbinol. For the $\Sigma\alpha_2^H$ value, cyclopentanol, cyclohexanol, and cycloheptanol each exhibit a value of 0.32, whereas the value for cyclopropyl carbinol was determined to be 0.36. This difference is probably not statistically significant.

Comparison of two of the six carbon aldehydes, namely 2-ethylbutanal (Table 2) with the previously published results for hexanal [7] show that the calculated values of 3.61 and 3.62 for the $\log L^{16}$ value are more in agreement with the published value for hexanal of 3.36 indicating that the value of 2.82 (Table 2) for 2-ethylbutanal (calculated intercept) may not be completely reliable. Comparing the calculated descriptors for 2-methyl-cyclohexanol (Table 2) with published results for the similar alcohol, cyclohexanol [7], reveal close agreement between the π_2^H values of 0.48 and 0.54, respectively and the $\Sigma\alpha_2^H$ values of 0.27 and 0.32, respectively. Any differences in the descriptor values are likely due to a combination of the difference in structure between the two compounds as well as minor errors associated with the methods of calculation.

Justification of the algebraic method of back calculation is illustrated with allyl formate. By MLRA, the π_2^H descriptor has a value of 0.77 when the y -intercept is calculated and 0.76 when the y -intercept is forced through zero. By comparison, the algebraically calculated value for allyl formate is

Table 2
Summary of newly calculated solute descriptor values

Solute	y-intercept	R_2	π_2^H	$\Sigma\alpha_2^H$	Log L^{16}	adj R^2	Standard error
Cyclopropyl carbinol							
calculated intercept	−0.003(0.007)		0.54(0.02)	0.36(0.01)		0.9972	0.02
intercept=0	0		0.54(0.01)	0.36(0.01)		0.9972	0.02
2-Methylcyclohexanol							
calculated intercept	−0.009(0.005)		0.49(0.01)	0.27(0.01)		0.9982	0.01
intercept=0	0		0.48(0.01)	0.27(0.01)		0.9980	0.01
Prop-2-yne-1-ol							
calculated intercept	−0.075(0.02)		0.50(0.04)	0.69(0.02)		0.9912	0.05
intercept=0	0		0.43(0.04)	0.68(0.03)		0.9879	0.06
2-Ethyl butanal							
calculated intercept	0.43(0.06)				2.82(0.10)	0.9388	0.03
intercept=0	0				3.61(0.01)	0.8632	0.05
algebraic calculation					3.62(0.10)		
Allyl formate							
calculated intercept	−0.002(0.010)		0.77(0.01)			0.9890	0.03
intercept=0	0		0.76(0.05)			0.9890	0.03
algebraic calculation			0.76(0.05)				
Ethylidene diacetate							
calculated intercept	0.11(0.09)		1.06(0.02)		3.35(0.14)	0.9884	0.03
intercept=0 (elimination	0		1.08(0.01)		3.52(0.02)	0.9881	0.03
of $\alpha_1\Sigma\alpha_2^H$ and r_1R_2 terms;							
insignificant)	0		1.07(0.01)		3.54(0.02)	0.9816	0.04
Cyclohexyl acetate							
calculated intercept	0.17(0.03)				4.15(0.06)	0.9899	0.02
intercept=0	0				4.47(0.01)	0.9839	0.03
algebraic calculation					4.48(0.04)		
1,3-Dioxolane							
calculated intercept	0.14(0.05)		0.72(0.01)		2.11(0.08)	0.9923	0.02
intercept=0	0		0.74(0.01)		2.33(0.08)	0.9910	0.02
4-Methyl-1,3-dioxolane							
calculated intercept	0.13(0.04)		0.63(0.01)		2.42(0.07)	0.9912	0.02
intercept=0	0		0.65(0.01)		2.62(0.01)	0.9896	0.02
4,5-Dimethyl-1,3-dioxolane							
calculated intercept	0.11(0.05)		0.59(0.01)		2.87(0.08)	0.9872	0.02
intercept=0	0		0.61(0.01)		3.04(0.01)	0.9858	0.02
1,1-Diisopropoxyethane							
calculated intercept	−0.01(0.06)		0.37(0.01)		3.97(0.11)	0.9766	0.02
intercept=0	0		0.37(0.00)		3.96(0.01)	0.9766	0.02
Di(2-ethyl-1-butyl)ether							
calculated intercept	−0.04(0.02)		0.21(0.02)			0.8501	0.02
intercept=0 (elimination	0		0.17(0.01)			0.8101	0.03
of $\alpha_1\Sigma\alpha_2^H$ and r_1R_2 terms;							
insignificant)							
algebraic calculation			0.17(0.03)				

Table 2. Continued

Solute	y-intercept	R_2	π_2^H	$\Sigma\alpha_2^H$	Log L^{16}	adj R^2	Standard error
<i>n</i> -Butyl vinyl ether							
calculated intercept	0.008(0.004)		0.35(0.01)			0.9885	0.01
intercept=0	0		0.35(0.00)			0.9876	0.01
algebraic calculation			0.36(0.05)				
Isobutyl vinyl ether							
calculated intercept	0.03(0.01)		0.30(0.01)			0.9795	0.02
intercept=0	0		0.33(0.00)			0.9671	0.02
algebraic calculation			0.35(0.04)				
2-Ethyl-1-hexyl vinyl ether							
calculated intercept	-0.002(0.009)		0.34(0.01)			0.9544	0.03
intercept=0	0		0.34(0.00)			0.9544	0.03
algebraic calculation			0.33(0.05)				
4-Hydroxy-4-methylpentan-2-one							
calculated intercept	-0.008(0.016)			0.19(0.01)		0.8605	0.04
intercept=0	0			0.19(0.00)		0.8597	0.04
algebraic calculation	0.18(0.05)						
2-Methoxyethyl vinyl ether							
calculated intercept	0.004(0.01)		0.67(0.01)			0.9931	0.02
intercept=0	0		0.67(0.00)			0.9931	0.02
algebraic calculation			0.68(0.05)				
Di(2-ethoxyethyl) ether							
calculated intercept	0.008(0.012)		0.76(0.01)			0.9872	0.03
intercept=0	0		0.77(0.01)			0.9870	0.03
algebraic calculation			0.77(0.06)				

0.76; as a result, all values determined by these approaches are in excellent agreement.

4. Conclusion

It has been demonstrated that back calculation of solute descriptors utilized in the LSER developed by Abraham and coworkers can be performed on several solutes as long as two criteria exist. First, the McReynold's gas chromatographic retention data set must contain enough information on several phases for a specific solute to make back calculation statistically reliable. Second, the calculated dependent variable must be sufficiently large to permit back calculation of accurate solute descriptor values, either by MLRA or algebraic calculation.

Finally, comparison of solute descriptor values determined by back calculation with values already published for homologous compounds shows this method to be reliable under the appropriate circumstances.

Acknowledgements

The work reported herein was performed in partial fulfillment of degree requirements for the Ph.D. degree from Northern Illinois University (B.K.C.).

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