Journal of Chromatography, 644 (1993) 95–139
Elsevier Science Publishers B.V., Amsterdam

CHROM. 25 120

Hydrogen bonding

XXVII. Solvation parameters for functionally substituted aromatic compounds and heterocyclic compounds, from gas–liquid chromatographic data

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(Received January 22nd, 1993)

ABSTRACT

The truncated solvation equation $\log SP = c + rR_2 + l \log L^{16}$ has been applied to a very large number of sets of gas–liquid chromatographic data on non-polar stationary phases. Here, $\log SP$ can be $\log V_G$ or can be the retention index I. R_2 is the excess molar refraction of the solute and c, r and l are constants. A set of solutes of known $\log L^{16}$ values is used to construct the equation, and then further values of $\log L^{16}$ can be obtained for any solute of known $\log SP$ value. In this way, new $\log L^{16}$ values for over 1000 solutes have been obtained. Then knowing $\log L^{16}$, and R_2, the equation $\log SP = c + rR_2 + s\pi_2^H + l \log L^{16}$ (s is a constant) can be applied to GLC data on polar non-acidic stationary phases, and the dipolarity/polarisability parameter, π_2^H determined similarly. Values of π_2^H for over 700 compounds are reported, including those for functionally substituted aromatic compounds and heterocyclic compounds. It is shown that π_2^H is a blend of dipolarity/polarisability, and cannot simply be calculated from solute dipole moments.

INTRODUCTION

We have recently shown [1–8] that the general solvation equation,

$$\log SP = c + rR_2 + s\pi_2^H + a\alpha_2^H + b\beta_2^H + l \log L^{16} \quad (1)$$

can be used to describe numerous processes in which a series of solutes are distributed between the gas phase and some condensed phase. These processes include gas–liquid chromatography (GLC) [1–5], gas–solid chromatography [6], the solubility of gases and vapours in polymers [7], and the solubility of gases and vapours in soya-bean oil [8]. The dependent variable in eqn. 1 can be $\log L$ or $\log K$, where L (or K) is the Ostwald solubility coefficient or gas–liquid partition coefficient, or $\log V_G$ where V_G is the specific retention volume at the column temperature, or $\log V_G^0$ the specific retention volume corrected to 273 K, or even $\log \tau$ where τ is the adjusted relative retention time. All these dependent variables will give rise to the same coefficients in eqn. 1 except for the constant term, c. The retention index, I, can also be used in place of $\log SP$, but now all the characteristic constants c, r, s, a, b and l will alter. Thus values of I cannot be used to characterise GLC stationary phases, but are very useful in the determination of descriptors, as we shall see later.

The explanatory variables, or descriptors, in eqn. 1 have been described before [1–10]. In brief they are: R_2 the solute excess molar refraction [9], π_2^H the solute dipolarity/polarisability, α_2^H the effective or summation solute hydrogen-bond acidity, β_2^H the effective or summation

0021-9673/93/$06.00

solute hydrogen-bond basicity, and log L^{16} where L^{16} is the solute gas–liquid partition coefficient on hexadecane at 298 K [1–5,9]. How general is the application of eqn. 1 depends in part on the availability of the descriptors, or solute parameters, used in the equation. There is no problem with R_2, which can be obtained from refractive index measurements on liquids at 293 K [10], or which can be calculated for solutes that are solid at 293 K, since R_2 is very nearly an additive property. However, the other four descriptors in eqn. 1 must be obtained by experiment, or by comparison to closely related compounds where possible. We have previously described the determination of π_2^H and log L^{16} for a wide variety of mostly aliphatic solutes [1], and for alkylaromatic solutes [5], and we now consider the very important class of functionally substituted aromatic compounds. During the course of this work we have also obtained π_2^H and log L^{16} values for a number of other compounds, and so we give these results as well.

The GLC stationary phases we shall consider are all either neutral or hydrogen-bond bases, so that the $b\beta_2^H$ term in eqn. 1 is redundant. Note that the b constant refers to the stationary phase acidity, the complementary property to solute hydrogen-bond basicity. Hence eqn. 1 will be reduced to eqn. 2

$$\log SP = c + rR_2 + s\pi_2^H + a\alpha_2^H + l \log L^{16} \quad (2)$$

For rather non-polar phases, such as squalane or apiezon, the π_2^H term is not significant, leaving

$$\log SP = c + rR_2 + a\alpha_2^H + l \log L^{16} \quad (3)$$

Now the a constant for such phases will be small or not significant, and so if α_2^H is known or can be estimated, then knowing R_2 and the constants in eqn. 3 it is possible to calculate log L^{16} for solutes with a known log SP value. Our method, as before [1,5] is thus to set up equations of the type of eqn. 3, to obtain the constants c, r, a and l, and then to obtain log L^{16} values by back-calculation. Retention index values can be used as log SP, leading to equations of the form,

$$I = c' + r'R_2 + a'\alpha_2^H + l' \log L^{16} \quad (4)$$

but the procedure is identical to that using eqn. 3.

If now GLC phases are chosen that are polar (but still non-acidic) such as Carbowax or esters, eqn. 1 will take the form of eqn. 2 or, in the case of log $SP = I$

$$I = c' + r'R_2 + s'\pi_2^H + a'\alpha_2^H + l' \log L^{16} \quad (5)$$

Once the constants in eqn. 2 or eqn. 5 have been established with solutes of known descriptors [1–5], then knowing R_2, α_2^H and log L^{16} (as above), the π_2^H parameter can be calculated for a variety of solutes of known log SP or of known I value.

RESULTS

There is a large amount of literature data on retention volumes or retention indices of aromatic compounds, including the extensive work of Korhonen and co-workers [11–19] the work of De Ligny *et al.* [20] and much other work on non-polar and polar stationary phases [21–97]. In addition there is an extensive compilation of GLC data that was also used [98].

A start was made on data obtained with rather non-polar stationary phases, for which eqn. 3 or eqn. 4 could be applied to calculate new values of log L^{16}. Some restrictions were placed on the data sets that were used. Generally, for sets that covered a wide range of compound type, at least some fifteen solutes were needed in the set. A few exceptions were made when solutes of similar compound type were involved. Secondly, data sets that yielded regression equations with poor fits were excluded. An estimate of the expected error in any calculated log L^{16} value can be obtained from the ratios S.D./l or S.D./l', where l and l' are the constants in eqn. 3 and eqn. 4, and S.D. is the overall standard deviation in the regression equation. In the event, some 75 data sets that conformed to eqn. 3 or eqn. 4 were considered. Once these data sets had been analyzed, the calculated log L^{16} values were averaged, and the entire analysis repeated. This had the effect of including more data points in a number of regressions, but the overall quality of the regression equations remained practically the same. Thus for the data of Bark and Clarke [38] on phenols chromatographed on OV-1 at 403 K, the successive equations were,

$$\log \tau = -1.901 + 0.453R_2 + 0.422 \log L^{16} \quad (6)$$
$$n = 11 \quad \rho = 0.9964 \quad \text{S.D.} = 0.039$$

$$\log \tau = -1.931 + 0.483R_2 + 0.427 \log L^{16} \quad (7)$$
$$n = 16 \quad \rho = 0.9967 \quad \text{S.D.} = 0.031$$

In these equations, n is the number of data points, ρ is the overall correlation constant, and S.D. is the standard deviation in the independent variable. The ratio S.D./l is 0.073 in eqn. 7, this being the estimate of the average error in the log L^{16} back-calculated values. For many data sets this ratio was rather smaller. Thus for the extensive results of Dutoit [95], the second round of analysis gave,

$$I/10 = 6.669 + 8.918R_2 + 20.002 \log L^{16} \quad (8)$$
$$n = 138 \quad \rho = 0.9995 \quad \text{S.D.} = 0.449$$

so that S.D./l' = 0.025 units. In eqn. 8 $I/10$ is used only for computing convenience. The only extensive set of literature data for which little use could be made was that of Peng *et al.* [81], yielding the regression equation,

$$I/10 = 6.317 + 9.129\pi_2^H + 9.596\alpha_2^H + 20.018 \log L^{16} \quad (9)$$
$$n = 156 \quad \rho = 0.9988 \quad \text{S.D.} = 1.524$$

Although Peng *et al.*'s results are for non-polar stationary phases, the present analysis suggests that a significant amount of polarity is associated with the phase. Furthermore, the quite large S.D./l' value of 0.076 (when combined with the necessity of requiring both π_2^H and a_2^H parameters) precluded any considerable use of Peng *et al.*'s results.

In Table I are given calculated log L^{16} values for over 1000 compounds, together with the number of values that have been averaged (No.), the average itself, the standard deviation in the log L^{16} value (S.D.) and the maximum and minimum calculated log L^{16} values. Also in Table I are values of the solute parameter R_2 needed for the calculation of log L^{16} via eqn. 3 or eqn. 4. A reasonable number of log L^{16} values in Table I are averages of three or more determinations: these can be regarded as reasonably firm values, since further experimental results will not be expected to alter the log L^{16} values to any extent. However, log L^{16} values for which only one datum is available, Table I, must be regarded, for the moment, as provisional. The experimental error in log L^{16} can be assessed from results on solutes for which (say) ten or more values have been averaged. There are 39 such solutes for which S.D. averages out as 0.057 log units, and for the functionally substituted benzenes only, there are 10 solutes for which S.D. averages as 0.038 log units. This is in accord with typical regression equations, where S.D./l or S.D./l' is around 0.04 or 0.05 log units.

It is of some interest to test whether or not the log L^{16} values can be calculated by a simple additive scheme. In Table II are functional group increments as $\Delta \log L^{16}$ obtained as,

$$\Delta \log L^{16} = \log L^{16}(\text{PhX}) - 2.786 \quad (10)$$

where 2.786 is log L^{16} for benzene itself. These substituent values, together with the value for benzene can then be used to calculate log L^{16} for a variety of disubstituted benzenes. For non-interacting substituents, the log L^{16} values are reasonably additive, for example in the case of the following *m*- and *p*-substituted benzenes; Me/Me, Me/Et, Et/Et, Me/F, F/F, Me/Cl, Cl/Cl, Me/Br, Br/Br, Me/I, I/I, Me/OMe, F/OMe, Cl/OMe, OMe/OMe, Me/CHO, Me/$COCH_3$, Me/NH_2, Me/NO_2, and Me/OH. However for *o*-substituted benzenes, additivity does not usually apply, and for *m*- and *p*-substituted benzenes with interacting substituents, additivity does not apply either, *e.g.*: NO_2/NH_2, CN/NH_2, Cl/OH, NO_2/OH, etc. Hence the additivity principle can be used to predict log L^{16} values for *m*- and *p*-methyl derivatives of functional groups, and for some halogen derivatives as well, but cannot be used as a general method for the prediction of log L^{16} values.

However, our previous conclusion, that log L^{16} increases regularly along an homologous series, except possibly for the first one or two members, applies to the *n*-alkyl benzoates, see Table I. For the ten solutes from *n*-propyl benzoate to *n*-dodecyl benzoate,

$$\log L^{16} = 4.1733 + 0.51005n(\text{C}) \quad (11)$$
$$n = 10 \quad r = 0.9999 \quad \text{S.D.} = 0.0067$$

TABLE I

CALCULATED VALUES OF LOG L^{16}

Solute	R_2	No.	Average	S.D.	Max	Min
Cyclopentane	0.263	5	2.477	0.030	2.515	2.433
Cyclohexane	0.305	14	2.964	0.106	3.202	2.734
Methylcyclohexane	0.244	5	3.323	0.046	3.395	3.278
Ethylcyclohexane	0.263	3	3.877	0.062	3.936	3.812
Cyclohexylcyclohexane	0.531	1	6.434			
Cycloheptane	0.350	6	3.704	0.040	3.778	3.659
Cyclooctane	0.413	6	4.329	0.065	4.460	4.279
Cyclononane	0.432	1	4.829			
Cyclodecane	0.474	4	5.340	0.014	5.353	5.322
Cycloundecane	0.517	1	5.761			
Cyclododecane	0.559	1	6.190			
Cyclotetradecane	0.644	1	7.363			
trans-Hydrindane	0.439	3	4.467	0.015	4.479	4.450
cis-Hydrindane	0.439	4	4.635	0.023	4.662	4.610
Adamantane	0.667	4	5.095	0.069	5.186	5.040
trans-Decalin	0.467	9	4.984	0.066	5.120	4.915
cis-Decalin	0.544	7	5.156	0.050	5.237	5.095
cis-2-Methyldecalin	0.540	1	5.550			
2-Methylbut-2-ene	0.159	2	2.226	0.051	2.262	2.190
2-Methylpent-2-ene	0.156	2	2.588	0.029	2.608	2.567
Cyclohexene	0.359	1	3.021			
1-Methylcyclohexene	0.391	1	3.483			
3-Methylcyclohexene	0.360	1	3.379			
4-Methylcyclohexene	0.347	1	3.372			
Cycloheptene	0.414	1	3.626			
Cyclooctene	0.460	1	4.119			
Cyclohexa-1,3-diene	0.515	1	2.917			
Cyclohexa-1,4-diene	0.501	1	3.132			
Cyclohepta-1,3-diene	0.615	1	3.607			
Cycloocta-1,5-diene	0.603	1	4.300			
Cyclohepta-1,3,5-triene	0.764	1	3.442			
Cycloocta-1,3,5,7-tetraene	0.804	1	3.884			
α-Pinene	0.446	1	4.200			
Dicyclopentadiene	0.712	1	4.651			
1-Fluorohexane	0.000	1	2.951			
1-Fluorooctane	−0.020	1	3.850			
Fluorocyclohexane	0.232	1	3.215			
1-Chlorooctane	0.191	2	4.772	0.058	4.813	4.731
Chlorocyclohexane	0.448	3	4.016	0.034	4.047	3.980
Bromocyclohexane	0.615	3	4.395	0.015	4.413	4.386
Iodocyclohexane	0.904	2	4.785	0.018	4.798	4.772
1-Chlorocyclohexene	0.530	1	3.990			
1-Bromocyclohexene	0.700	1	4.350			
1-Bromo-4-methylcyclohexene	0.650	1	4.669			
1-Iodocyclohexene	1.000	1	4.838			
Dibromomethane	0.714	3	2.886	0.027	2.905	2.855
Tribromomethane	0.974	3	3.784	0.056	3.816	3.719
Fluorotrichloromethane	0.207	2	1.995	0.091	2.059	1.930
1,1-Difluorotetrachloroethane	0.230	1	2.970			
1,2-Difluorotetrachloroethane	0.227	2	2.929	0.100	3.000	2.858
Methyl cyclohexyl ether	0.296	1	3.861			
1,2-Dimethoxyethane	0.116	1	2.565			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2,5-Diethoxytetrahydrofuran	0.126	1	3.335			
1,8-Cineole	0.383	1	4.290			
Propenal	0.324	1	1.656			
trans-But-2-ene-1-al	0.387	1	2.570			
trans-Hex-2-ene-1-al	0.404	1	3.400			
trans-Hept-2-ene-1-al	0.400	1	3.897			
Carvone	0.674	1	5.330			
Butan-2,3-dione	0.220	1	1.639			
Acetylacetone	0.401	2	2.918	0.206	3.064	2.772
Ethyl trimethylacetate	0.000	1	3.481			
2-Methoxyethyl acetate	0.166	1	3.290			
2-Ethoxyethylacetate	0.099	1	3.747			
Diethylmalonate	0.112	1	4.472			
Cyanocyclohexane	0.410	1	4.333			
Isopentylamine	0.194	1	3.058			
Cyclohexylamine	0.326	2	3.796	0.057	3.836	3.755
3-Methylcyclohexylamine	0.383	1	4.125			
Di-*n*-propylamine	0.124	2	3.351	0.030	3.372	3.329
Di-isobutylamine	0.046	1	3.901			
Di-*n*-pentylamine	0.099	1	4.570			
Triethylamine	0.101	2	3.040	0.052	3.077	3.003
Tri-*n*-propylamine	0.066	1	4.229			
1-Nitrohexane	0.203	4	4.416	0.008	4.426	4.409
Nitrocyclohexane	0.441	3	4.826	0.108	4.951	4.762
Dimethylformamide	0.367	1	3.173			
Diethylformamide	0.305	1	3.995			
Dibutylformamide	0.255	1	5.927			
Dimethylacetamide	0.363	1	3.717			
Dimethylpropanamide	0.340	1	3.720			
Dimethylisobutanamide	0.310	1	4.371			
Dimethylpivalamide	0.270	1	4.623			
Heptan-2-ol	0.188	4	3.838	0.050	3.886	3.768
2-Ethoxyethanol	0.237	1	2.815			
trans-Hex-2-ene-1-ol	0.294	1	3.510			
trans-Hept-2-ene-1-ol	0.281	1	4.010			
trans-Oct-2-ene-1-ol	0.270	1	4.520			
Dodecafluoroheptan-1-ol	−0.640	1	3.089			
Dimethylsulphoxide	0.522	2	3.459	0.031	3.481	3.437
Tetramethylsilicon	0.000	2	1.778	0.021	1.793	1.763
Cyclopropylbenzene	0.806	1	4.479			
Diphenylmethane	1.220	8	6.313	0.044	6.364	6.218
2-Methyldiphenylmethane	1.220	3	6.812	0.013	6.823	6.797
3-Methyldiphenylmethane	1.220	3	6.771	0.001	6.772	6.770
4-Methyldiphenylmethane	1.220	3	6.864	0.008	6.873	6.858
1,1-Diphenylethane	1.289	3	6.506	0.006	6.512	6.501
1,2-Diphenylethane	1.200	8	6.764	0.031	6.797	6.702
1,4-Diphenylbutane	1.200	3	7.882	0.011	7.894	7.872
Biphenyl	1.360	17	6.014	0.106	6.128	5.647
2-Methylbiphenyl	1.330	5	6.058	0.088	6.188	5.939
3-Methylbiphenyl	1.370	7	6.591	0.046	6.666	6.551
4-Methylbiphenyl	1.370	9	6.612	0.048	6.666	6.522

(Continued on p. 100)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2-Ethylbiphenyl	1.270	4	6.403	0.109	6.567	6.341
3-Ethylbiphenyl	1.370	3	6.954	0.008	6.961	6.945
4-Ethylbiphenyl	1.370	3	7.098	0.005	7.102	7.093
2,3-Dimethylbiphenyl	1.405	3	6.632	0.010	6.641	6.621
2,4-Dimethylbiphenyl	1.354	3	6.576	0.012	6.587	6.563
2,5-Dimethylbiphenyl	1.354	3	6.519	0.018	6.537	6.502
2,6-Dimethylbiphenyl	1.405	3	6.139	0.016	6.151	6.121
3,4-Dimethylbiphenyl	1.434	3	7.235	0.003	7.238	7.232
3,5-Dimethylbiphenyl	1.406	3	7.030	0.010	7.040	7.020
2,2′-Dimethylbiphenyl	1.286	4	6.168	0.087	6.298	6.117
2,3′-Dimethylbiphenyl	1.330	3	6.491	0.016	6.506	6.474
2,4′-Dimethylbiphenyl	1.342	3	6.588	0.012	6.600	6.576
3,3′-Dimethylbiphenyl	1.380	4	7.080	0.046	7.148	7.049
3,4′-Dimethylbiphenyl	1.380	3	7.126	0.006	7.132	7.120
4,4′-Dimethylbiphenyl	1.380	6	7.159	0.069	7.228	7.070
2-Isopropylbiphenyl	1.270	3	6.407	0.009	6.413	6.397
3-Isopropylbiphenyl	1.370	3	7.152	0.006	7.159	7.148
4-Isopropylbiphenyl	1.370	3	7.362	0.002	7.365	7.361
Triphenylmethane	1.830	2	8.545	0.208	8.692	8.398
o-Terphenyl	2.000	2	8.244	0.221	8.400	8.088
m-Terphenyl	2.040	1	9.530			
p-Terphenyl	2.040	1	9.689			
o-Quaterphenyl	2.700	1	11.145			
m-Quaterphenyl	2.740	1	12.584			
p-Quaterphenyl	2.740	1	13.039			
1,3,5-Triphenylbenzene	2.440	4	12.787	0.074	12.882	12.702
trans-Stilbene	1.700	5	7.469	0.148	7.650	7.238
cis-Stilbene	1.600	2	6.474	0.015	6.484	6.463
α-Methylstilbene (*cis*, *trans*?)	1.650	2	7.402	0.013	7.411	7.393
1-Ethylnaphthalene	1.371	2	6.136	0.041	6.165	6.107
2-Ethylnaphthalene	1.331	3	6.140	0.030	6.168	6.108
1-Propylnaphthalene	1.370	1	6.495			
2-Propylnaphthalene	1.330	1	6.563			
2-Isopropylnaphthalene	1.330	1	6.400			
1-Butylnaphthalene	1.370	1	6.977			
2-Butylnaphthalene	1.330	1	7.065			
1-Isobutylnaphthalene	1.370	1	6.653			
2-Isobutylnaphthalene	1.330	1	6.764			
2-*sec*.-Butylnaphthalene	1.330	1	6.797			
2-*tert*.-Butylnaphthalene	1.330	1	6.703			
1,3,7-Trimethylnaphthalene	1.390	1	6.733			
2,3,5-Trimethylnaphthalene	1.469	3	6.935	0.019	6.951	6.914
2,3,6-Trimethylnaphthalene	1.430	4	6.871	0.014	6.892	6.862
1-Phenylnaphthalene	1.950	1	8.217			
2-Phenylnaphthalene	1.950	2	8.717	0.022	8.732	8.701
2-Benzylnaphthalene	1.950	3	8.562	0.065	8.621	8.493
1,4-Dihydronaphthalene	1.096	1	5.040			
5-Methyltetralin	0.940	2	5.860	0.033	5.883	5.836
6-Methyltetralin	0.900	2	5.751	0.017	5.763	5.739
2,6-Dimethyltetralin	0.900	2	5.997	0.013	6.006	5.987
Acenaphthene	1.604	9	6.469	0.034	6.541	6.415
Acenaphthylene	1.750	5	6.175	0.067	6.241	6.069
1,2,2*a*,3,4,6-Hexahydroacenaphthylene	1.340	1	6.005			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
1-Methylacenaphthylene	1.750	2	6.818	0.004	6.821	6.815
Fluorene	1.588	14	6.922	0.152	7.162	6.512
1-Methylfluorene	1.588	4	7.443	0.191	7.578	7.162
2-Methylfluorene	1.588	4	7.426	0.180	7.554	7.162
9-Methylfluorene	1.588	2	7.090	0.005	7.093	7.086
9-Ethylfluorene	1.588	1	7.459			
9-Propylfluorene	1.588	1	8.435			
9-Butylfluorene	1.588	1	8.760			
9-Hexylfluorene	1.588	1	9.338			
Azulene	1.340	9	5.707	0.124	5.844	5.415
1-Methylazulene	1.340	1	6.379			
5-Methylazulene	1.340	1	6.385			
6-Methylazulene	1.340	1	6.442			
4,6,8-Trimethylazulene	0.340	1	7.641			
Anthracene	2.290	13	7.568	0.086	7.692	7.391
9,10-Dihydroanthracene	1.400	1	7.526			
1,2,3,4,5,6,7,8-Octahydroanthracene	1.188	1	7.687			
Decahydroanthracene	0.705	2	7.073	0.187	7.205	6.940
1-Methylanthracene	2.290	1	8.332			
2-Methylanthracene	2.290	3	8.184	0.114	8.280	8.058
9-Methylanthracene	2.290	3	8.438	0.120	8.512	8.299
9,10-Dimethylanthracene	2.290	1	9.283			
9-Phenylanthracene	2.900	1	10.265			
Phenanthrene	2.055	13	7.632	0.091	7.759	7.463
9,10-Dihydrophenanthrene	1.690	1	7.483			
1,2,3,4-Tetrahydrophenanthrene	1.606	1	7.813			
1,2,3,4,5,6,7,8-Octahydrophenanthrene	1.145	3	7.842	0.062	7.909	7.787
1-Methylphenanthrene	2.055	4	8.408	0.104	8.525	8.274
2-Methylphenanthrene	2.055	2	8.307	0.027	8.326	8.288
3-Methylphenanthrene	2.055	2	8.286	0.028	8.305	8.266
4-Methylphenanthrene	2.055	2	8.394	0.029	8.414	8.373
9-Methylphenanthrene	2.055	2	8.392	0.027	8.411	8.373
2-Ethylphenanthrene	2.055	1	8.838			
9-Ethylphenanthrene	2.055	1	8.825			
1,8-Dimethylphenanthrene	2.055	1	9.097			
2,7-Dimethylphenanthrene	2.055	1	8.889			
3,6-Dimethylphenanthrene	2.055	1	8.848			
9-Methyl-10-ethylphenanthrene	2.055	1	9.500			
9-Propylphenanthrene	2.055	1	9.216			
9-Isopropylphenanthrene	2.055	1	9.083			
9,10-Diethylphenanthrene	2.055	1	9.739			
1-Methyl-7-isopropylphenanthrene	2.055	1	9.759			
9,10-Dimethyl-3-ethylphenanthrene	2.055	1	10.149			
1-Phenylphenanthrene	2.665	1	11.100			
9-Phenylphenanthrene	2.665	1	10.663			
9-Methyl-10-phenylphenanthrene	2.665	1	10.967			
4H-Cyclopenta[*def*]phenanthrene	2.417	6	8.126	0.106	8.248	8.002
7-Benz[*de*]anthrene	2.530	1	10.758			
Fluoranthene	2.377	11	8.827	0.083	8.962	8.739
1,2,3,10*b*-Tetrahydrofluoranthene	1.900	1	8.271			
Benzo[*a*]fluorene	2.622	11	9.404	0.073	9.504	9.308

(Continued on p. 102)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
11-Methylbenzo[*a*]fluorene	2.622	1	9.501			
Benzo[*b*]fluorene	2.622	5	9.520	0.069	9.590	9.435
Benzo[*c*]fluorene	2.622	2	9.525	0.092	9.590	9.460
Pyrene	2.808	14	8.833	0.068	8.964	8.746
4,5-Dihydropyrene	2.360	1	8.503			
4,5,9,10-Tetrahydropyrene	1.970	1	8.639			
1,2,3,6,7,8-Hexahydropyrene	1.950	1	8.932			
1-Methylpyrene	2.808	5	9.541	0.073	9.624	9.462
2-Methylpyrene	2.808	2	9.502	0.031	9.524	9.480
3-Methylpyrene	2.808	6	9.510	0.047	9.597	9.473
4-Methylpyrene	2.808	2	9.493	0.018	9.506	9.480
1-Ethylpyrene	2.808	1	9.973			
1-Butylpyrene	2.808	1	10.846			
2,7-Dimethylpyrene	2.808	1	10.002			
Cyclopenta[*cd*]pyrene	3.200	2	10.150	0.013	10.159	10.141
Benz[*a*]anthracene	2.992	10	10.291	0.063	10.376	10.162
4,5,6-Trihydrobenz[*de*]anthracene	2.360	1	9.711			
1-Methylbenz[*a*]anthracene	2.992	1	10.763			
2-Methylbenz[*a*]anthracene	2.992	1	10.745			
3-Methylbenz[*a*]anthracene	2.992	1	10.830			
4-Methylbenz[*a*]anthracene	2.992	2	10.909	0.016	10.920	10.898
5-Methylbenz[*a*]anthracene	2.992	1	10.891			
7-Methylbenz[*a*]anthracene	2.992	4	11.096	0.117	11.256	10.997
6-Methylbenz[*a*]anthracene	2.992	1	10.857			
8-Methylbenz[*a*]anthracene	2.992	1	10.857			
9-Methylbenz[*a*]anthracene	2.992	1	10.826			
11-Methylbenz[*a*]anthracene	2.992	1	10.714			
12-Methylbenz[*a*]anthracene	2.992	2	10.905	0.009	10.911	10.898
1,12-Dimethylbenz[*a*]anthracene	2.992	1	11.427			
7,12-Dimethylbenz[*a*]anthracene	2.992	4	11.753	0.154	11.960	11.621
Benzo[*c*]phenanthrene	3.000	4	10.020	0.066	10.081	9.930
Naphthacene	2.847	4	10.748	0.338	11.236	10.458
5,12-Dihydronaphthacene	2.255	1	10.066			
Chrysene	3.027	11	10.334	0.097	10.466	10.129
1-Methylchrysene	3.027	2	10.993	0.012	11.001	10.984
2-Methylchrysene	3.027	2	10.884	0.004	10.886	10.881
3-Methylchrysene	3.027	2	10.849	0.016	10.860	10.837
4-Methylchrysene	3.027	2	10.937	0.006	10.941	10.933
5-Methylchrysene	3.027	2	10.905	0.004	10.907	10.902
6-Methylchrysene	3.027	2	10.934	0.001	10.934	10.933
Triphenylene	3.000	6	10.355	0.078	10.454	10.235
Dodecahydrotriphenylene	1.537	1	10.475			
1-Methyltriphenylene	3.000	1	10.818			
1,3-Dimethyltriphenylene	3.000	1	11.291			
1,6,11-Trimethyltriphenylene	3.000	1	11.702			
1,3,6,11-Tetramethyltriphenylene	3.000	1	12.160			
Perylene	3.256	12	12.053	0.113	12.294	11.902
Benz[*a*]fluoranthene	3.194	1	11.608			
Benz[*b*]fluoranthene	3.194	8	11.609	0.088	11.719	11.479
Benz[*j*]fluoranthene	3.194	2	11.496	0.033	11.519	11.473
Benzo[*k*]fluoranthene	3.194	4	11.607	0.093	11.723	11.521
Benz[*mno*]fluoranthene	3.194	4	9.913	0.031	9.932	9.866
Benzo[*ghi*]fluoranthene	3.194	4	9.879	0.084	9.956	9.802

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
Benzofluoranthene 2,3	3.194	2	11.654	0.060	11.696	11.611
3-Methylcholanthrene	3.264	4	12.482	0.155	12.604	12.261
20-Methylcholanthrene	3.264	3	12.503	0.148	12.604	12.333
Indeno[1,2,3-*cd*]pyrene	3.610	2	12.690	0.227	12.850	12.529
Benzo[*a*]pyrene	3.625	10	11.715	0.082	11.828	11.526
3,4-Benzpyrene	3.625	7	11.765	0.094	11.896	11.590
Benz[*e*]pyrene	3.625	4	11.656	0.148	11.865	11.519
Dibenz[*ac*]anthracene	4.000	5	12.998	0.209	13.223	12.773
Pentacene	4.000	1	12.531			
Dibenz[*ah*]anthracene	4.000	5	12.960	0.174	13.202	12.786
Dibenz[*aj*]anthracene	4.000	1	13.028			
Picene	4.000	4	13.068	0.217	13.376	12.910
Benzo[*b*]chrysene	4.000	2	12.865	0.019	12.878	12.851
Benzo[*ghi*]perylene	4.073	5	13.264	0.484	14.070	12.892
1,2,3,4-Dibenzpyrene	4.621	2	14.347	0.416	14.641	14.053
1,2,4,5-Dibenzpyrene	4.621	1	15.077			
3,4,8,9-Dibenzpyrene	4.621	1	15.236			
3,4,9,10-Dibenzpyrene	4.621	1	15.236			
Dibenz[*cd,jk*]pyrene Anthanthrene	4.621	1	13.234			
Dibenz[*def,mno*]chrysene	4.621	2	12.807	0.002	12.808	12.805
2,3-Dihydrodibenz[*def,mno*]chrysene	4.000	1	13.036			
Coronene	4.236	2	14.712	0.636	15.161	14.262
1,1′-Binaphthyl	2.680	1	10.110			
1,2′-Binaphthyl	2.680	1	10.612			
2,2′-Binaphthyl	2.680	1	11.161			
Fluorobenzene	0.477	10	2.788	0.014	2.810	2.759
1,2-Difluorobenzene	0.390	1	3.620			
1,4-Difluorobenzene	0.384	1	2.766			
1,2,4,5-Tetrafluorobenzene	0.234	1	2.637			
Pentafluorobenzene	0.154	1	2.578			
Hexafluorobenzene	0.088	2	2.515	0.018	2.528	2.502
2-Fluorotoluene	0.491	2	3.338	0.021	3.352	3.323
3-Fluorotoluene	0.485	2	3.332	0.023	3.348	3.315
4-Fluorotoluene	0.488	2	3.366	0.026	3.384	3.347
Benzotrifluoride	0.225	2	2.894	0.008	2.899	2.888
Chlorobenzene	0.718	15	3.657	0.047	3.742	3.515
1,2-Dichlorobenzene	0.872	5	4.518	0.020	4.544	4.498
1,3-Dichlorobenzene	0.847	6	4.410	0.027	4.434	4.374
1,4-Dichlorobenzene	0.825	5	4.435	0.030	4.455	4.383
1,2,3-Trichlorobenzene	1.030	5	5.419	0.067	5.462	5.302
1,2,4-Trichlorobenzene	0.980	5	5.248	0.032	5.282	5.198
1,3,5-Trichlorobenzene	0.980	5	5.045	0.026	5.083	5.020
1,2,3,4-Tetrachlorobenzene	1.180	4	6.171	0.020	6.200	6.154
1,2,3,5-Tetrachlorobenzene	1.160	5	5.922	0.057	5.980	5.839
1,2,4,5-Tetrachlorobenzene	1.160	5	5.926	0.053	5.980	5.851
Pentachlorobenzene	1.330	4	6.716	0.109	6.852	6.599
Hexachlorobenzene	1.490	3	7.624	0.078	7.674	7.534
2-Chlorotoluene	0.762	5	4.173	0.014	4.185	4.150
3-Chlorotoluene	0.736	5	4.179	0.011	4.195	4.166
4-Chlorotoluene	0.705	5	4.205	0.016	4.225	4.188
2,4-Dichlorotoluene	0.921	2	4.951	0.018	4.963	4.938

(Continued on p. 104)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2,5-Dichlorotoluene	0.888	2	4.984	0.021	4.999	4.969
2,6-Dichlorotoluene	0.919	2	4.948	0.018	4.961	4.935
3,4-Dichlorotoluene	0.900	1	5.089			
2,3,4-Trichlorotoluene	1.080	2	5.980	0.033	6.003	5.957
2,3,5-Trichlorotoluene	1.060	2	5.772	0.004	5.774	5.769
2,3,6-Trichlorotoluene	1.100	1	5.759			
2,4,5-Trichlorotoluene	1.060	2	5.805	0.033	5.828	5.781
2,4,6-Trichlorotoluene	1.060	2	5.605	0.031	5.627	5.583
2,3,4,5-Tetrachlorotoluene	1.230	2	6.744	0.031	6.766	6.722
2,3,4,6-Tetrachlorotoluene	1.230	1	6.729			
2,3,5,6-Tetrachlorotoluene	1.230	2	6.513	0.018	6.526	6.500
Pentachlorotoluene	1.390	2	7.391	0.011	7.398	7.383
2-Chloro-*p*-xylene	0.775	4	4.700	0.047	4.733	4.630
2,3-Dichloro-*p*-xylene	0.949	3	5.646	0.056	5.710	5.605
2,5-Dichloro-*p*-xylene	0.949	3	5.485	0.039	5.519	5.442
2,3,5-Trichloro-*p*-xylene	1.117	3	6.371	0.046	6.408	6.320
Benzyl chloride	0.821	4	4.384	0.115	4.557	4.320
4-Methylbenzyl chloride	0.830	1	4.840			
2-Chlorobenzyl chloride	0.931	1	5.101			
4-Chlorobenzyl chloride	0.920	1	5.640			
2-Chloro-4-methylbenzyl chloride	0.931	1	5.651			
3-Chloro-4-methylbenzyl chloride	0.944	1	5.692			
1,4-Bis(chloromethyl)benzene	1.032	1	5.857			
Benzal chloride	0.916	1	5.151			
4-Chlorobenzal chloride	1.024	1	5.978			
Benzotrichloride	1.005	1	5.450			
4-Chlorobenzotrichloride	1.113	1	6.101			
2-Chlorostyrene	0.983	1	4.785			
Bromobenzene	0.882	14	4.041	0.033	4.077	3.965
1,2-Dibromobenzene	1.190	1	5.456			
1,3-Dibromobenzene	1.170	1	5.327			
1,4-Dibromobenzene	1.150	1	5.324			
1,3,5-Tribromobenzene	1.450	1	6.307			
2-Bromotoluene	0.923	3	4.559	0.014	4.575	4.548
3-Bromotoluene	0.896	3	4.577	0.016	4.589	4.559
4-Bromotoluene	0.879	3	4.586	0.007	4.593	4.579
Benzyl bromide	1.014	4	4.672	0.013	4.689	4.660
2-Bromo-1-phenylethane	0.974	3	5.170	0.013	5.181	5.156
2-Bromobiphenyl	1.592	1	6.435			
1-Bromonaphthalene	1.326	1	6.682			
2-Bromonaphthalene	1.286	1	6.678			
Iodobenzene	1.188	9	4.502	0.038	4.558	4.460
1,2-Diiodobenzene	1.860	1	6.395			
1,3-Diiodobenzene	1.830	1	6.377			
1,4-Diiodobenzene	1.800	1	6.255			
2-Iodotoluene	1.223	1	5.043			
3-Iodotoluene	1.210	1	5.036			
4-Iodotoluene	1.190	1	5.048			
Methylphenylether	0.708	15	3.890	0.054	4.000	3.769
Ethylphenylether	0.681	4	4.242	0.021	4.260	4.218
2-Methylanisole	0.725	2	4.339	0.063	4.383	4.294
3-Methylanisole	0.709	1	4.393			
4-Methylanisole	0.699	1	4.406			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2,3-Dimethylanisole	0.775	1	5.084			
2,4-Dimethylanisole	0.739	1	4.913			
2,5-Dimethylanisole	0.739	1	4.859			
2,6-Dimethylanisole	0.674	1	4.641			
3,4-Dimethylanisole	0.757	1	5.208			
3,5-Dimethylanisole	0.728	1	5.053			
2-Ethylanisole	0.741	1	4.656			
3-Ethylanisole	0.717	1	4.920			
4-Ethylanisole	0.728	1	4.963			
2-Propylanisole	0.740	1	5.200			
3-Propylanisole	0.720	1	5.524			
4-Propylanisole	0.720	1	5.614			
4-Allylanisole	0.815	1	5.475			
2-Fluoroanisole	0.600	1	3.887			
3-Fluoroanisole	0.571	1	3.865			
4-Fluoroanisole	0.571	2	3.904	0.054	3.942	3.865
2-Chloroanisole	0.883	4	4.847	0.108	5.009	4.787
3-Chloroanisole	0.825	3	4.685	0.052	4.741	4.637
4-Chloroanisole	0.838	5	4.802	0.099	4.955	4.702
2,3-Dichloroanisole	1.000	3	5.901	0.059	5.953	5.836
2,4-Dichloroanisole	1.000	4	5.734	0.068	5.787	5.639
2,5-Dichloroanisole	1.000	4	5.685	0.064	5.734	5.596
2,6-Dichloroanisole	1.030	4	5.273	0.017	5.287	5.252
3,4-Dichloroanisole	0.960	3	5.762	0.032	5.793	5.729
3,5-Dichloroanisole	0.940	3	5.544	0.027	5.570	5.516
2,3,4-Trichloroanisole	1.130	3	6.720	0.027	6.751	6.703
2,3,5-Trichloroanisole	1.120	3	6.506	0.050	6.548	6.451
2,3,6-Trichloroanisole	1.150	3	6.153	0.040	6.177	6.107
2,4,5-Trichloroanisole	1.120	4	6.499	0.051	6.541	6.428
2,4,6-Trichloroanisole	1.150	4	5.929	0.066	5.982	5.844
3,4,5-Trichloroanisole	1.080	3	6.563	0.025	6.591	6.543
2,3,4,5-Tetrachloroanisole	1.280	3	7.318	0.068	7.396	7.268
2,3,4,6-Tetrachloroanisole	1.310	4	6.790	0.040	6.835	6.748
2,3,5,6-Tetrachloroanisole	1.300	3	6.798	0.035	6.830	6.760
Pentachloroanisole	1.420	4	7.566	0.105	7.696	7.441
2-Chloro-5-methylanisole	0.880	2	5.438	0.016	5.450	5.426
4-Chloro-3-methylanisole	0.840	2	5.343	0.004	5.345	5.340
4-Bromoanisole	0.992	2	5.187	0.023	5.203	5.170
4-Iodoanisole	1.286	1	5.616			
Methyl benzyl ether	0.645	3	4.238	0.008	4.246	4.231
Ethyl benzyl ether	0.629	1	4.524			
Dibenzyl ether	1.210	2	7.316	0.016	7.327	7.305
Diphenyl ether	1.216	3	6.287	0.028	6.315	6.259
1,2-Dimethoxybenzene	0.832	2	4.925	0.054	4.963	4.887
1,3-Dimethoxybenzene	0.816	1	5.022			
4-Methylveratrole	0.830	1	5.588			
3-Chloroveratrole	0.960	1	5.580			
4-Chloroveratrole	0.960	1	5.775			
3,4-Dichloroveratrole	1.090	1	6.506			
3,5-Dichloroveratrole	1.080	1	6.305			
3,6-Dichloroveratrole	1.090	1	5.956			

(Continued on p. 106)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
4,5-Dichloroveratrole	1.090	1	6.662			
3,4,5-Trichloroveratrole	1.240	1	7.291			
3,4,6-Trichloroveratrole	1.240	1	6.725			
Tetrachloroveratrole	1.380	1	7.647			
Benzaldehyde	0.820	9	4.008	0.039	4.083	3.967
2-Methylbenzaldehyde	0.870	2	4.559	0.030	4.580	4.538
3-Methylbenzaldehyde	0.840	4	4.548	0.015	4.565	4.528
4-Methylbenzaldehyde	0.862	4	4.592	0.042	4.654	4.564
2,4-Dimethylbenzaldehyde	0.929	2	5.170	0.028	5.189	5.150
2,5-Dimethylbenzaldehyde	0.900	2	5.106	0.018	5.118	5.093
3,4-Dimethylbenzaldehyde	0.890	2	5.367	0.042	5.397	5.337
4-Isopropylbenzaldehyde	0.859	1	5.294			
Furfural	0.690	1	3.262			
Phthalaldehyde	0.990	2	5.542	0.334	5.778	5.305
Terephthalaldehyde	1.030	2	5.500	0.379	5.768	5.232
Phenylacetaldehyde	0.755	2	4.344	0.004	4.346	4.341
3-Phenylpropanal	0.750	2	4.913	0.007	4.918	4.908
Acetophenone	0.818	7	4.501	0.020	4.540	4.483
4-Methylacetophenone	0.842	1	5.081			
2-Methoxyacetophenone	0.892	1	5.992			
3-Methoxyacetophenone	0.902	1	6.153			
4-Methoxyacetophenone	0.916	1	6.500			
Ethylphenylketone	0.804	2	4.971	0.009	4.977	4.964
n-Propylphenylketone	0.797	2	5.343	0.017	5.355	5.331
Benzylmethylketone	0.748	3	4.726	0.077	4.815	4.679
1-Phenylbutan-2-one	0.746	2	5.138	0.011	5.146	5.130
4-Phenylbutan-2-one	0.746	2	5.245	0.013	5.254	5.235
1,4-Naphthoquinone	1.080	1	6.341			
2-Methyl-1,4-naphthoquinone	1.080	1	6.886			
Anthraquinone	1.405	2	8.593	0.000	8.593	8.593
Phenanthraquinone	1.410	2	9.395	0.010	9.402	9.388
Anthrone	1.372	2	8.879	0.009	8.885	8.872
Methyl benzoate	0.733	7	4.704	0.088	4.835	4.634
Ethyl benzoate	0.689	4	5.075	0.091	5.211	5.014
Propyl benzoate	0.675	1	5.718			
Butyl benzoate	0.668	1	6.210			
Pentyl benzoate	0.663	1	6.718			
Hexyl benzoate	0.657	1	7.230			
Heptyl benzoate	0.653	1	7.739			
Octyl benzoate	0.647	1	8.248			
Nonyl benzoate	0.640	1	8.763			
Decyl benzoate	0.632	1	9.276			
Undecyl benzoate	0.630	1	9.786			
Dodecyl benzoate	0.627	1	10.299			
Methyl 2-methylbenzoate	0.772	3	5.053	0.022	5.076	5.032
Methyl 3-methylbenzoate	0.754	3	5.204	0.023	5.218	5.178
Methyl 4-methylbenzoate	0.730	3	5.248	0.013	5.260	5.234
Methyl 2,4-dimethylbenzoate	0.770	2	5.620	0.021	5.634	5.605
Methyl 2,5-dimethylbenzoate	0.800	2	5.559	0.025	5.576	5.541
Methyl 3,4-dimethylbenzoate	0.760	2	5.959	0.078	6.014	5.904
Methyl 4-isopropylbenzoate	0.760	2	5.977	0.038	6.004	5.950
Methyl 2-fluorobenzoate	0.576	1	4.719			
Methyl 3-fluorobenzoate	0.556	1	4.620			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
Methyl 4-fluorobenzoate	0.556	1	4.620			
Methyl 2-chlorobenzoate	0.817	2	5.702	0.102	5.774	5.630
Methyl 4-chlorobenzoate	0.797	1	5.620			
Methyl 2,4-dichlorobenzoate	0.950	1	6.353			
Methyl 2,5-dichlorobenzoate	0.950	1	6.372			
Methyl 2,3,6-trichlorobenzoate	1.050	1	6.923			
Methyl 4-methoxybenzoate	0.830	1	5.848			
Methyl 2-methoxy-3,6-dichlorobenzoate	1.050	1	6.917			
Benzyl benzoate	1.264	1	7.873			
Phenyl acetate	0.661	1	4.414			
2-Methylphenyl acetate	0.661	2	4.924	0.110	5.002	4.846
3-Methylphenyl acetate	0.660	1	4.871			
4-Methylphenyl acetate	0.660	1	4.900			
Benzyl acetate	0.798	1	5.012			
2-Methylbenzyl acetate	0.840	2	5.413	0.185	5.543	5.282
4-Methylbenzyl acetate	0.800	1	5.318			
2,4-Dimethylbenzyl acetate	0.840	2	5.934	0.170	6.054	5.813
2,5-Dimethylbenzyl acetate	0.850	2	5.875	0.182	6.003	5.746
3,4-Dimethylbenzyl acetate	0.810	2	6.077	0.203	6.220	5.933
2-Phenylethyl acetate	0.788	1	5.364			
Methyl phenylacetate	0.700	2	4.879	0.023	4.895	4.862
Ethyl phenylacetate	0.660	1	5.522			
Ethyl cinnamate	1.107	1	6.322			
Dimethyl phthalate	0.780	1	6.051			
Dimethyl isophthalate	0.830	1	6.482			
Dimethyl terephthalate	0.850	1	6.453			
Dimethyl methylterephthalate	0.850	1	6.856			
Benzonitrile	0.742	9	4.039	0.045	4.141	3.990
2-Methylbenzonitrile	0.780	1	4.478			
3-Methylbenzonitrile	0.762	1	4.561			
4-Methylbenzonitrile	0.740	1	4.600			
2-Chlorobenzonitrile	0.890	1	4.847			
3-Chlorobenzonitrile	0.870	1	4.712			
4-Chlorobenzonitrile	0.850	1	4.757			
Phenylacetonitrile	0.751	5	4.700	0.055	4.779	4.639
cis-Cinnamonitrile	1.098	1	5.339			
trans-Cinnamonitrile	1.186	1	5.597			
2-Methyl-*cis*-cinnamonitrile	1.140	1	5.768			
2-Methyl-*trans*-cinnamonitrile	1.230	1	6.025			
2-Chloro-*cis*-cinnamonitrile	1.250	1	5.941			
2-Chloro-*trans*-cinnamonitrile	1.330	1	6.352			
2-Bromo-*cis*-cinnamonitrile	1.410	1	6.364			
2-Bromo-*trans*-cinnamonitrile	1.500	1	6.745			
2-Methoxy-*cis*-cinnamonitrile	1.220	1	6.304			
2-Methoxy-*trans*-cinnamonitrile	1.300	1	6.640			
4-Methyl-*cis*-cinnamonitrile	1.100	1	5.936			
4-Methyl-*trans*-cinnamonitrile	1.190	1	6.193			
4-Chloro-*cis*-cinnamonitrile	1.210	1	6.234			
4-Chloro-*trans*-cinnamonitrile	1.290	1	6.545			
4-Methoxy-*cis*-cinnamonitrile	1.200	1	6.537			
4-Methoxy-*trans*-cinnamonitrile	1.280	1	6.849			

(Continued on p. 108)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
4-Trifluoromethyl-*cis*-cinnamonitrile	0.710	1	5.222			
4-Trifluoromethyl-*trans*-cinnamonitrile	0.800	1	5.504			
Aniline	0.955	13	3.934	0.032	3.993	3.866
o-Toluidine	0.966	8	4.442	0.042	4.494	4.364
m-Toluidine	0.946	8	4.463	0.043	4.536	4.417
p-Toluidine	0.923	8	4.452	0.040	4.510	4.404
2-Ethylaniline	0.962	3	4.829	0.083	4.921	4.761
3-Ethylaniline	0.940	2	4.840	0.064	4.885	4.794
4-Ethylaniline	0.942	3	4.895	0.099	4.986	4.789
2,3-Dimethylaniline	1.010	2	5.088	0.009	5.094	5.081
2,4-Dimethylaniline	0.950	4	4.983	0.016	4.997	4.961
2,5-Dimethylaniline	0.962	3	4.966	0.049	5.006	4.912
2,6-Dimethylaniline	0.972	6	5.028	0.019	5.049	4.998
3,4-Dimethylaniline	0.960	3	5.089	0.063	5.161	5.047
3,5-Dimethylaniline	0.956	2	5.072	0.001	5.072	5.071
2,6-Diethylaniline	0.987	1	6.342			
2-Vinylaniline	1.230	1	4.783			
3-Vinylaniline	1.210	1	4.975			
4-Vinylaniline	1.210	1	4.908			
2-Fluoroaniline	0.744	3	3.771	0.085	3.861	3.693
3-Fluoroaniline	0.749	2	3.988	0.090	4.051	3.924
4-Fluoroaniline	0.760	3	4.007	0.028	4.032	3.977
2-Chloroaniline	1.033	3	4.674	0.016	4.692	4.660
3-Chloroaniline	1.053	3	4.909	0.016	4.924	4.893
4-Chloroaniline	1.060	2	4.889	0.015	4.899	4.878
2-Bromoaniline	1.070	3	5.104	0.011	5.115	5.093
3-Bromoaniline	1.128	3	5.304	0.009	5.314	5.298
4-Bromoaniline	1.190	3	5.276	0.011	5.288	5.268
2-Iodoaniline	1.290	3	5.574	0.020	5.591	5.552
3-Iodoaniline	1.414	3	5.739	0.011	5.747	5.726
4-Iodoaniline	1.530	3	5.695	0.033	5.731	5.665
2-Cyanoaniline	1.067	1	5.018			
3-Cyanoaniline	1.077	1	5.380			
4-Cyanoaniline	1.087	1	5.639			
2-Methoxyaniline	0.988	3	4.818	0.066	4.865	4.742
3-Methoxyaniline	1.027	3	5.023	0.036	5.049	4.982
4-Methoxyaniline	1.050	3	4.949	0.049	4.984	4.893
2-Ethoxyaniline	0.888	1	5.203			
3-Ethoxyaniline	0.927	1	5.430			
4-Ethoxyaniline	0.950	2	5.357	0.001	5.357	5.356
2-Nitroaniline	1.180	3	5.627	0.022	5.652	5.609
3-Nitroaniline	1.200	1	5.880			
4-Nitroaniline	1.220	1	6.343			
o-Phenylenediamine	1.260	2	4.845	0.005	4.848	4.841
m-Phenylenediamine	1.280	1	4.893			
3-Fluoro-4-methylaniline	0.717	2	4.509	0.026	4.527	4.490
4-Fluoro-2-methylaniline	0.771	2	4.533	0.024	4.550	4.516
2,4-Difluoroaniline	0.549	2	3.843	0.043	3.873	3.812
2,5-Difluoroaniline	0.538	2	3.898	0.049	3.932	3.863
2,3-Dichloroaniline	1.136	2	5.652	0.006	5.656	5.647
2,4-Dichloroaniline	1.140	2	5.650	0.006	5.654	5.645
3,4-Dichloroaniline	1.160	2	5.944	0.015	5.954	5.933
2-Bromo-4-methylaniline	1.084	1	5.579			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
3-Bromo-4-methylaniline	1.142	1	5.541			
2,5-Dimethoxyaniline	1.065	2	5.954	0.012	5.962	5.945
2-Methoxy-5-aminoaniline	1.318	1	5.948			
N-Methylaniline	0.948	8	4.478	0.024	4.508	4.448
N-Ethylaniline	0.945	4	4.811	0.042	4.846	4.752
N-Propylaniline	0.921	3	5.324	0.013	5.338	5.313
N-Butylaniline	0.908	2	5.836	0.007	5.841	5.831
N-Isopentylaniline	0.890	2	6.183	0.015	6.193	6.172
2-Methyl-N-methylaniline	0.959	3	4.885	0.027	4.915	4.861
3-Methyl-N-methylaniline	0.939	3	4.917	0.066	4.993	4.870
4-Methyl-N-methylaniline	0.916	2	4.983	0.041	5.012	4.954
2-Methyl-N-ethylaniline	0.956	2	5.213	0.008	5.219	5.207
3-Methyl-N-ethylaniline	0.936	2	5.322	0.006	5.326	5.317
4-Methyl-N-ethylaniline	0.913	2	5.346	0.005	5.349	5.342
2-Chloro-N-methylaniline	1.026	2	5.025	0.010	5.032	5.018
4-Chloro-N-methylaniline	1.053	2	5.445	0.002	5.446	5.443
N,N-Dimethylaniline	0.957	8	4.701	0.037	4.748	4.644
N,N-Diethylaniline	0.953	5	5.287	0.074	5.392	5.207
N-Methyl-N-ethylaniline	0.955	2	4.953	0.012	4.961	4.944
2-Methyl-N,N-dimethylaniline	1.090	4	4.608	0.069	4.708	4.559
3-Methyl-N,N-dimethylaniline	0.993	4	5.144	0.116	5.228	4.978
4-Methyl-N,N-dimethylaniline	0.940	5	5.188	0.028	5.211	5.146
2,4-Dimethyl-N,N-dimethylaniline	0.970	1	5.070			
2,6-Dimethyl-N,N-dimethylaniline	0.990	1	4.921			
4-*tert.*-Butyl-N,N-dimethylaniline	0.944	1	6.337			
3-Methyl-N,N-diethylaniline	0.936	2	5.804	0.006	5.808	5.800
4-Methyl-N,N-diethylaniline	0.989	2	5.759	0.008	5.764	5.753
2-Chloro-N,N-dimethylaniline	1.035	2	5.110	0.007	5.115	5.105
4-Bromo-N,N-dimethylaniline	1.230	2	6.046	0.018	6.059	6.033
1-Naphthylamine	1.670	1	6.490			
2-Naphthylamine	1.670	1	6.540			
2-Aminoanthracene	2.635	4	9.300	0.103	9.452	9.225
Benzylamine	0.829	1	4.319			
Dibenzylamine	1.316	1	7.596			
Diphenylamine	1.700	2	7.086	0.006	7.090	7.082
2,2′-Bipyridyl	1.384	5	6.385	0.025	6.428	6.366
Nitrobenzene	0.871	9	4.557	0.032	4.618	4.524
2-Nitrotoluene	0.866	3	4.878	0.027	4.900	4.848
3-Nitrotoluene	0.874	3	5.097	0.028	5.122	5.067
4-Nitrotoluene	0.870	3	5.154	0.025	5.178	5.128
2-Nitrobiphenyl	1.580	3	7.452	0.115	7.582	7.365
3-Nitrobiphenyl	1.680	3	8.031	0.093	8.132	7.949
4-Nitrobiphenyl	1.680	3	8.190	0.103	8.265	8.072
4-Nitro-*p*-terphenyl	2.300	1	11.583			
1-Nitronaphthalene	1.600	1	6.991			
2-Nitronaphthalene	1.600	1	7.176			
2-Nitrofluorene	1.850	1	9.126			
1-Fluoro-3-nitrobenzene	0.737	1	4.441			
1-Chloro-2-nitrobenzene	1.020	2	5.235	0.011	5.243	5.227
1-Chloro-3-nitrobenzene	1.000	2	5.206	0.051	5.242	5.170
1-Chloro-4-nitrobenzene	0.980	2	5.220	0.002	5.221	5.218

(Continued on p. 110)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2,3-Dichloronitrobenzene	1.180	1	5.837			
2,4-Dichloronitrobenzene	1.130	1	5.752			
2,5-Dichloronitrobenzene	1.130	1	5.726			
2,6-Dichloronitrobenzene	1.180	1	5.650			
3,4-Dichloronitrobenzene	1.130	1	5.843			
3,5-Dichloronitrobenzene	1.130	1	5.575			
2,3,4-Trichloronitrobenzene	1.330	1	6.432			
2,3,5-Trichloronitrobenzene	1.310	1	6.156			
2,3,6-Trichloronitrobenzene	1.330	1	6.189			
2,4,5-Trichloronitrobenzene	1.310	1	6.247			
2,4,6-Trichloronitrobenzene	1.310	1	5.978			
3,4,5-Trichloronitrobenzene	1.310	1	6.333			
2,3,4,5-Tetrachloronitrobenzene	1.480	1	6.875			
2,3,4,6-Tetrachloronitrobenzene	1.480	1	6.637			
2,3,5,6-Tetrachloronitrobenzene	1.480	1	6.606			
Pentachloronitrobenzene	1.640	1	7.261			
Benzamide	0.990	1	5.767			
Dimethyl phenylacetamide	0.920	1	6.899			
Phenol	0.805	12	3.766	0.059	3.885	3.682
o-Cresol	0.840	11	4.218	0.051	4.293	4.112
m-Cresol	0.822	10	4.310	0.036	4.348	4.240
p-Cresol	0.820	10	4.312	0.038	4.387	4.271
2-Ethylphenol	0.831	6	4.612	0.076	4.726	4.509
3-Ethylphenol	0.810	5	4.741	0.085	4.873	4.652
4-Ethylphenol	0.800	6	4.737	0.080	4.862	4.632
2,3-Dimethylphenol	0.850	6	4.952	0.023	4.977	4.919
2,4-Dimethylphenol	0.843	6	4.770	0.020	4.795	4.742
2,5-Dimethylphenol	0.840	5	4.774	0.022	4.796	4.739
2,6-Dimethylphenol	0.860	4	4.680	0.062	4.753	4.605
3,4-Dimethylphenol	0.830	6	4.980	0.032	5.019	4.935
3,5-Dimethylphenol	0.820	6	4.856	0.053	4.947	4.798
2-*n*-Propylphenol	0.822	3	4.951	0.062	4.996	4.880
3-*n*-Propylphenol	0.789	3	5.117	0.025	5.143	5.094
4-*n*-Propylphenol	0.793	3	5.185	0.034	5.221	5.153
2-Isopropylphenol	0.842	4	4.816	0.090	4.921	4.733
3-Isopropylphenol	0.811	2	4.951	0.066	4.998	4.904
4-Isopropylphenol	0.791	3	4.984	0.055	5.042	4.933
2-Methyl-3-ethylphenol	0.850	1	5.228			
2-Methyl-4-ethylphenol	0.843	2	5.161	0.011	5.168	5.153
2-Methyl-5-ethylphenol	0.840	1	5.149			
3-Methyl-4-ethylphenol	0.830	1	5.295			
3-Methyl-5-ethylphenol	0.820	2	5.215	0.046	5.247	5.182
3-Methyl-6-ethylphenol	0.840	1	5.030			
4-Methyl-2-ethylphenol	0.843	2	5.052	0.026	5.070	5.033
4-Methyl-3-ethylphenol	0.830	1	5.419			
2,3,4-Trimethylphenol	0.860	1	5.544			
2,3,5-Trimethylphenol	0.860	2	5.334	0.042	5.363	5.304
2,3,6-Trimethylphenol	0.870	2	5.270	0.063	5.314	5.225
2,4,5-Trimethylphenol	0.850	1	5.386			
2,4,6-Trimethylphenol	0.860	5	5.133	0.039	5.185	5.091
3,4,5-Trimethylphenol	0.830	1	5.568			
2-*n*-Butylphenol	0.806	1	5.473			
3-*n*-Butylphenol	0.800	1	5.590			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
4-*n*-Butylphenol	0.796	2	5.640	0.055	5.679	5.601
2-*sec.*-Butylphenol	0.819	2	5.050	0.086	5.111	4.989
4-*sec.*-Butylphenol	0.800	2	5.332	0.161	5.445	5.218
2-*tert.*-Butylphenol	0.823	2	5.021	0.195	5.159	4.883
4-*tert.*-Butylphenol	0.810	3	5.264	0.097	5.340	5.155
2,4-Diethylphenol	0.840	1	5.375			
2,5-Diethylphenol	0.820	1	5.440			
2,6-Diethylphenol	0.860	1	5.199			
3,5-Diethylphenol	0.820	1	5.500			
2-Methyl-6-propylphenol	0.860	1	5.524			
4-Methyl-2-propylphenol	0.820	1	5.419			
3-Methyl-5-propylphenol	0.810	1	5.634			
2-Methyl-4-isopropylphenol	0.824	1	5.464			
3-Methyl-5-isopropylphenol	0.810	1	5.429			
4-Methyl-2-isopropylphenol	0.822	1	5.198			
3,4-Dimethyl-6-ethylphenol	0.850	1	5.678			
2,3,4,5-Tetramethylphenol	0.870	1	6.099			
2,3,5,6-Tetramethylphenol	0.880	2	5.788	0.172	5.909	5.666
2(1-Methylbutyl)phenol	0.820	1	5.524			
4(1-Methylbutyl)phenol	0.790	1	5.921			
4-*tert.*-Pentylphenol	0.810	1	5.775			
2-Ethyl-5-propylphenol	0.810	1	5.880			
4-Methyl-2,6-diethylphenol	0.860	1	5.722			
Pentamethylphenol	0.900	1	6.725			
2(1-Methylpentyl)phenol	0.820	1	5.965			
4(1-Methylpentyl)phenol	0.790	1	6.383			
2,6-Dipropylphenol	0.820	1	5.910			
2,6-Di-isopropylphenol	0.860	1	5.637			
2,4-Dimethyl-6-*tert.*-butylphenol	0.860	1	5.859			
2(1-Methylhexyl)phenol	0.820	1	6.479			
4(1-Methylhexyl)phenol	0.790	1	6.914			
2(1-Methylheptyl)phenol	0.820	1	6.935			
4(1-Methylheptyl)phenol	0.790	1	7.377			
4-Methyl-2,6-di-*tert.*-butylphenol	0.860	1	6.255			
Thymol	0.822	2	5.381	0.134	5.476	5.286
Carvacrol	0.824	1	5.369			
4-Cyclohexylphenol	1.110	1	7.226			
2-Phenylphenol	1.550	1	7.227			
5,6,7,8-Tetrahydro-1-naphthol	1.043	1	6.624			
5,6,7,8-Tetrahydro-2-naphthol	1.020	1	6.747			
4-Indanol	0.980	1	5.820			
5-Indanol	0.960	1	5.879			
5-Methyl-4-indanol	0.990	1	6.236			
6-Methyl-4-indanol	0.980	1	6.280			
7-Methyl-4-indanol	0.990	1	6.328			
4-Methyl-5-indanol	1.000	1	6.230			
6-Methyl-5-indanol	0.980	1	6.280			
7-Methyl-5-indanol	0.960	1	6.355			
2-Fluorophenol	0.660	1	3.453			
3-Fluorophenol	0.667	2	3.842	0.004	3.844	3.839
4-Fluorophenol	0.670	2	3.844	0.016	3.855	3.833

(Continued on p. 112)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2-Chlorophenol	0.853	2	4.178	0.023	4.194	4.162
3-Chlorophenol	0.909	5	4.773	0.090	4.893	4.650
4-Chlorophenol	0.915	5	4.775	0.105	4.917	4.667
2-Bromophenol	1.037	1	4.526			
3-Bromophenol	1.060	2	5.144	0.083	5.202	5.085
4-Bromophenol	1.080	2	5.135	0.117	5.218	5.052
2-Iodophenol	1.360	1	4.964			
3-Iodophenol	1.370	1	5.528			
4-Iodophenol	1.380	1	5.492			
2,3-Dichlorophenol	0.960	2	4.989	0.049	5.024	4.954
2,4-Dichlorophenol	0.969	2	4.943	0.066	4.989	4.896
2,5-Dichlorophenol	0.960	2	4.939	0.059	4.980	4.897
2,6-Dichlorophenol	0.900	2	5.086	0.048	5.120	5.052
3,4-Dichlorophenol	1.020	2	5.708	0.182	5.837	5.579
3,5-Dichlorophenol	1.020	2	5.653	0.261	5.837	5.468
2,3,4-Trichlorophenol	1.070	2	5.772	0.221	5.928	5.615
2,3,5-Trichlorophenol	1.070	2	5.609	0.190	5.743	5.475
2,3,6-Trichlorophenol	1.010	2	5.718	0.140	5.817	5.619
2,4,5-Trichlorophenol	1.070	2	5.725	0.226	5.885	5.565
2,4,6-Trichlorophenol	1.010	2	5.664	0.204	5.808	5.519
3,4,5-Trichlorophenol	1.130	2	6.351	0.684	6.835	5.867
2,3,4,5-Tetrachlorophenol	1.170	2	6.353	0.573	6.758	5.947
2,3,4,6-Tetrachlorophenol	1.110	1	6.740			
2,3,5,6-Tetrachlorophenol	1.110	2	6.294	0.561	6.690	5.897
Pentachlorophenol	1.220	2	6.822	1.107	7.604	6.039
2-Chloro-5-methylphenol	0.930	1	4.354			
4-Chloro-2-methylphenol	0.890	1	5.246			
4-Chloro-3-methylphenol	0.920	1	5.290			
2,4-Dibromophenol	1.310	1	5.282			
2,6-Dibromophenol	1.270	1	5.608			
2-Methoxyphenol	0.837	3	4.449	0.096	4.548	4.356
3-Methoxyphenol	0.879	1	4.803			
4-Methoxyphenol	0.900	1	4.773			
2-Hydroxybenzaldehyde	0.962	1	4.539			
4-Hydroxybenzaldehyde	1.010	1	5.533			
2-Chloro-4-hydroxybenzaldehyde	1.130	1	6.495			
3-Chloro-4-hydroxybenzaldehyde	1.140	1	5.528			
2,3-Dichloro-4-hydroxybenzaldehyde	1.180	1	6.374			
2,5-Dichloro-4-hydroxybenzaldehyde	1.180	1	6.300			
2,6-Dichloro-4-hydroxybenzaldehyde	1.250	1	7.589			
3,5-Dichloro-4-hydroxybenzaldehyde	1.110	1	6.363			
2,3,5-Trichloro-4-hydroxybenzaldehyde	1.230	1	7.144			
2,3,6-Trichloro-4-hydroxybenzaldehyde	1.300	1	7.265			
Tetrachloro-4-hydroxybenzaldehyde	1.340	1	8.051			
Catechol	0.970	2	5.060	0.152	5.168	4.952
Resorcinol	0.980	6	6.216	0.276	6.585	5.750
Hydroquinone	1.000	6	5.937	0.253	6.296	5.585
4-Allyl-2-methoxyphenol	0.928	1	5.992			
4-Propyl-2-methoxyphenol	0.820	1	6.069			
2-*tert.*-Butyl-4-methoxyphenol	0.920	1	6.603			
2,6-Dimethoxyphenol	0.870	1	6.287			
4-Methyl-2,6-dimethoxyphenol	0.870	1	6.826			
4-Ethyl-2,6-dimethoxyphenol	0.870	1	7.127			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
4-Propyl-2,6-dimethoxyphenol	0.870	1	7.451			
2-Cyanophenol	0.920	1	4.531			
3-Cyanophenol	0.930	1	5.181			
4-Cyanophenol	0.940	1	5.420			
2-Nitrophenol	1.015	3	4.760	0.091	4.861	4.684
3-Nitrophenol	1.050	2	5.692	0.028	5.711	5.672
4-Nitrophenol	1.070	2	5.876	0.116	5.958	5.794
3-Methyl-2-nitrophenol	1.030	1	5.274			
2-Methyl-4-nitrophenol	1.100	1	6.324			
2-Methyl-5-nitrophenol	1.080	1	6.222			
2-Methyl-6-nitrophenol	1.050	1	5.300			
2,5-Dimethyl-4-nitrophenol	1.120	1	6.620			
2,6-Dimethyl-4-nitrophenol	1.120	1	6.605			
2,4-Dinitrophenol	1.280	1	6.041			
2,5-Dinitrophenol	1.260	1	5.959			
2,6-Dinitrophenol	1.220	1	6.189			
3,4-Dinitrophenol	1.320	1	5.953			
1-Naphthol	1.520	1	6.130			
2-Naphthol	1.520	1	6.200			
Benzyl alcohol	0.803	10	4.221	0.016	4.249	4.193
2-Methylbenzyl alcohol	0.850	2	4.659	0.117	4.742	4.576
3-Methylbenzyl alcohol	0.815	2	4.581	0.113	4.661	4.501
4-Methylbenzyl alcohol	0.810	2	4.584	0.136	4.680	4.488
2,4-Dimethylbenzyl alcohol	0.857	2	5.117	0.088	5.179	5.055
2,5-Dimethylbenzyl alcohol	0.868	2	5.119	0.080	5.175	5.062
3,4-Dimethylbenzyl alcohol	0.830	2	5.190	0.112	5.269	5.111
4-Isopropylbenzyl alcohol	0.804	2	5.119	0.189	5.252	4.985
1-Phenylethanol	0.784	2	4.394	0.007	4.399	4.389
2-Phenylethanol	0.811	6	4.628	0.043	4.713	4.601
3-Phenylpropan-1-ol	0.821	1	5.180			
2-Phenylpropan-2-ol	0.848	2	4.520	0.003	4.522	4.518
Phenylmethylsulphide	1.068	1	4.659			
Furan	0.369	1	1.830			
Benzofuran	0.888	3	4.355	0.024	4.378	4.330
Dibenzofuran	1.407	8	6.716	0.018	6.745	6.694
Dinaphtho[1,2-*b*;1′,2′-*d*]furan	3.230	1	11.734			
Xanthene	1.220	1	7.462			
Benzo[*kl*]xanthene	1.830	1	9.627			
Dibenzo[*c*,*kl*]xanthene	2.440	1	12.068			
Benzodioxane	0.874	1	4.971			
4-Phenyl-1,3-dioxane	0.857	1	6.081			
9-Fluorenone	1.342	1	7.840			
11-Benzo[*a*]fluorenone	1.950	1	10.323			
9-Xanthenone	1.430	2	8.116	0.004	8.118	8.113
Dibenzo-*p*-dioxin	1.290	1	7.045			
Trioxan	0.100	1	2.650			
Paraldehyde	0.136	1	3.169			
Pyridine	0.631	20	3.022	0.046	3.131	2.899
2-Methylpyridine	0.598	16	3.422	0.034	3.471	3.324
3-Methylpyridine	0.631	17	3.631	0.030	3.724	3.592
4-Methylpyridine	0.630	16	3.640	0.033	3.718	3.593

(Continued on p. 114)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2-Ethylpyridine	0.613	13	3.844	0.027	3.900	3.801
3-Ethylpyridine	0.640	12	4.093	0.034	4.170	4.025
4-Ethylpyridine	0.634	13	4.124	0.030	4.207	4.095
2,3-Dimethylpyridine	0.657	10	4.045	0.028	4.086	3.988
2,4-Dimethylpyridine	0.634	13	4.006	0.045	4.132	3.963
2,5-Dimethylpyridine	0.633	11	3.986	0.030	4.050	3.927
2,6-Dimethylpyridine	0.607	14	3.760	0.052	3.856	3.656
3,4-Dimethylpyridine	0.676	10	4.317	0.037	4.385	4.257
3,5-Dimethylpyridine	0.659	10	4.214	0.024	4.250	4.176
2-*n*-Propylpyridine	0.604	6	4.288	0.028	4.330	4.249
3-*n*-Propylpyridine	0.632	1	4.546			
4-*n*-Propylpyridine	0.627	6	4.597	0.030	4.632	4.555
4-Isopropylpyridine	0.625	1	4.449			
2-Methyl-4-ethylpyridine	0.639	3	4.442	0.015	4.459	4.432
2-Methyl-5-ethylpyridine	0.629	4	4.467	0.051	4.541	4.427
2-Methyl-6-ethylpyridine	0.613	5	4.102	0.063	4.156	3.994
3-Methyl-2-ethylpyridine	0.662	1	4.392			
3-Methyl-4-ethylpyridine	0.681	2	4.728	0.011	4.736	4.720
3-Methyl-5-ethylpyridine	0.664	1	4.622			
3-Methyl-6-ethylpyridine	0.638	1	4.398			
4-Methyl-2-ethylpyridine	0.639	3	4.376	0.009	4.384	4.366
4-Methyl-3-ethylpyridine	0.689	1	4.989			
2,3,4-Trimethylpyridine	0.703	4	4.688	0.018	4.706	4.664
2,3,5-Trimethylpyridine	0.687	5	4.524	0.081	4.613	4.394
2,3,6-Trimethylpyridine	0.674	6	4.308	0.070	4.376	4.178
2,4,5-Trimethylpyridine	0.686	4	4.630	0.042	4.687	4.592
2,4,6-Trimethylpyridine	0.634	13	4.324	0.065	4.513	4.246
3,4,5-Trimethylpyridine	0.690	1	4.939			
2-*n*-Butylpyridine	0.600	1	4.790			
4-*tert.*-Butylpyridine	0.631	3	4.742	0.008	4.750	4.734
2,5-Diethylpyridine	0.640	1	4.822			
2,6-Diethylpyridine	0.619	1	4.428			
3,4-Diethylpyridine	0.690	1	5.116			
3,5-Diethylpyridine	0.670	1	4.873			
2-Methyl-4-propylpyridine	0.600	1	4.889			
2-Methyl-5-propylpyridine	0.600	1	4.879			
2-Methyl-6-propylpyridine	0.620	1	4.571			
4-Methyl-2-propylpyridine	0.600	1	4.818			
4-Methyl-3-propylpyridine	0.680	1	5.128			
5-Methyl-2-propylpyridine	0.600	1	4.830			
4-Methyl-3-isopropylpyridine	0.680	1	4.995			
2,3-Dimethyl-4-ethylpyridine	0.703	2	5.078	0.070	5.127	5.028
2,3-Dimethyl-6-ethylpyridine	0.674	1	4.690			
2,4-Dimethyl-5-ethylpyridine	0.686	2	5.030	0.048	5.064	4.996
2,4-Dimethyl-6-ethylpyridine	0.634	2	4.646	0.004	4.648	4.643
2,5-Dimethyl-4-ethylpyridine	0.686	2	5.043	0.009	5.049	5.036
2,5-Dimethyl-6-ethylpyridine	0.674	2	4.672	0.045	4.704	4.640
2,6-Dimethyl-3-ethylpyridine	0.674	2	4.756	0.021	4.771	4.741
2,6-Dimethyl-4-ethylpyridine	0.634	2	4.736	0.019	4.749	4.722
3,4-Dimethyl-6-ethylpyridine	0.686	1	4.996			
3,5-Dimethyl-6-ethylpyridine	0.687	1	4.904			
2,3,4,5-Tetramethylpyridine	0.770	1	5.339			
2,3,4,6-Tetramethylpyridine	0.727	4	4.988	0.066	5.079	4.935

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2,3,5,6-Tetramethylpyridine	0.730	2	4.876	0.006	4.880	4.871
2-*n*-Pentylpyridine	0.600	2	5.270	0.014	5.280	5.260
4-*n*-Pentylpyridine	0.620	1	5.980			
2-Methyl-6-butylpyridine	0.620	1	5.042			
2-Ethyl-6-propylpyridine	0.620	1	4.924			
2-Methyl-4,5-diethylpyridine	0.690	1	5.443			
2-Methyl-4,6-diethylpyridine	0.640	2	5.078	0.023	5.094	5.061
2-Methyl-5,6-diethylpyridine	0.680	1	5.023			
4-Methyl-2,6-diethylpyridine	0.640	1	5.004			
2,6-Dimethyl-4-propylpyridine	0.630	1	5.200			
2-Isopropyl-3,6-dimethylpyridine	0.670	1	4.901			
2,3,6-Trimethyl-4-ethylpyridine	0.730	1	5.346			
2,4,6-Trimethyl-3-ethylpyridine	0.730	2	5.327	0.002	5.328	5.325
2,3,4-Triethylpyridine	0.710	1	5.726			
2,3,5-Triethylpyridine	0.700	1	5.458			
2,4,6-Triethylpyridine	0.640	1	5.463			
2,3-Dimethyl-4,6-diethylpyridine	0.740	1	5.659			
2,5-Dimethyl-4,6-diethylpyridine	0.740	1	5.614			
3,4-Dimethyl-2,6-diethylpyridine	0.750	1	5.643			
2(5-Nonyl)pyridine	0.570	1	6.560			
4(5-Nonyl)pyridine	0.600	1	7.380			
2-Benzylpyridine	1.222	1	7.250			
4-Benzylpyridine	1.244	1	7.730			
3,5-Diphenylpyridine	1.851	2	9.956	0.045	9.987	9.924
Cyclopenteno[*b*]pyridine	1.020	1	4.628			
2-Methylcyclopenteno[*b*]pyridine	1.020	1	4.813			
4-Methylcyclopenteno[*b*]pyridine	1.020	1	4.968			
7-Methylcyclopenteno[*b*]pyridine	1.020	1	4.769			
Cyclopenteno[*c*]pyridine	1.020	1	4.818			
3-Methylthiopyridine	1.040	1	4.760			
2-Fluoropyridine	0.489	2	3.106	0.076	3.159	3.052
3-Fluoropyridine	0.504	2	2.991	0.057	3.031	2.950
4-Fluoropyridine	0.500	1	2.934			
2-Chloropyridine	0.738	3	3.875	0.118	3.946	3.739
3-Chloropyridine	0.732	4	3.783	0.046	3.840	3.729
4-Chloropyridine	0.740	2	3.728	0.037	3.754	3.701
2-Bromopyridine	0.921	2	4.386	0.065	4.432	4.340
3-Bromopyridine	0.905	2	4.185	0.001	4.186	4.184
4-Bromopyridine	0.900	2	4.027	0.140	4.126	3.928
2-Iodopyridine	1.210	1	4.712			
3-Iodopyridine	1.210	1	4.635			
4-Iodopyridine	1.210	1	4.553			
3-Methoxypyridine	0.680	1	4.290	0.000	4.290	4.290
4-Methoxypyridine	0.680	1	4.279			
2-Acetylpyridine	0.730	1	4.478			
3-Acetylpyridine	0.795	1	4.880			
4-Acetylpyridine	0.771	1	4.660			
2-Cyanopyridine	0.734	2	4.441	0.213	4.591	4.290
3-Cyanopyridine	0.750	2	4.164	0.159	4.276	4.051
4-Cyanopyridine	0.750	3	4.033	0.121	4.155	3.913
2-Formylpyridine	0.768	1	4.031			

(Continued on p. 116)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
3-Formylpyridine	0.817	1	4.258			
β-Methylnicotinate	0.710	1	5.095			
2-Nitropyridine	0.890	1	4.667			
3-Nitropyridine	0.890	1	4.548			
4-Nitropyridine	0.890	1	4.327			
2-Chloro-5-nitropyridine	1.000	1	5.609			
2-Methoxy-5-nitropyridine	0.900	1	5.875			
2-Methoxy-3-nitropyridine	0.920	1	5.913			
Piperidine	0.422	2	3.304	0.008	3.310	3.298
N-Methylpiperidine	0.318	2	3.330	0.099	3.400	3.260
N-Ethylpiperidine	0.300	2	3.729	0.069	3.778	3.680
Quinoline	1.268	13	5.457	0.069	5.608	5.331
1,2,3,4-Tetrahydroquinoline	1.221	2	5.665	0.262	5.850	5.480
2-Methylquinoline	1.287	9	5.791	0.050	5.879	5.707
3-Methylquinoline	1.317	1	5.969			
4-Methylquinoline	1.335	8	6.126	0.055	6.242	6.060
6-Methylquinoline	1.309	9	5.988	0.049	6.057	5.897
7-Methylquinoline	1.305	7	5.992	0.026	6.017	5.941
8-Methylquinoline	1.313	10	5.801	0.061	5.862	5.683
2,3-Dimethylquinoline	1.370	1	6.330			
2,4-Dimethylquinoline	1.352	4	6.371	0.076	6.456	6.305
2,6-Dimethylquinoline	1.320	6	6.294	0.057	6.355	6.219
2,7-Dimethylquinoline	1.320	1	6.310			
2,4,6-Trimethylquinoline	1.390	1	6.854			
2,4,6,8-Tetramethylquinoline	1.440	1	6.860			
6-Phenylquinoline	1.878	2	9.010	0.057	9.050	8.969
Isoquinoline	1.211	11	5.595	0.062	5.708	5.466
1,2,3,4-Tetrahydroisoquinoline	1.016	1	5.170			
1-Methylisoquinoline	1.275	2	5.941	0.074	5.993	5.888
3-Methylisoquinoline	1.230	3	5.931	0.034	5.960	5.893
Benzo[*c*]quinoline	1.878	7	7.978	0.079	8.073	7.878
Benzo[*f*]quinoline	1.878	7	7.974	0.080	8.068	7.872
2-Methylbenzo[*f*]quinoline	1.878	1	8.373			
3-Methylbenzo[*f*]quinoline	1.878	4	8.314	0.097	8.409	8.184
Benzo[*h*]quinoline	1.878	7	7.797	0.045	7.861	7.759
Indeno[1,2,3-*ij*]isoquinoline	2.180	1	9.089			
Benzo[*lmn*]phenanthridine	2.488	1	9.299			
Acridine	2.356	8	7.644	0.089	7.751	7.462
9,10-Dihydroacridine	1.600	2	7.959	0.042	7.988	7.929
2-Methylacridine	2.356	4	8.252	0.095	8.341	8.130
3-Methylacridine	2.356	2	8.064	0.053	8.101	8.026
9-Methylacridine	2.356	1	8.512			
Benz[*a*]acridine	2.970	3	10.285	0.025	10.309	10.260
10-Methylbenz[*a*]acridine	2.970	1	10.782			
5,7-Dimethylbenz[*a*]acridine	2.970	1	11.459			
7,10-Dimethylbenz[*a*]acridine	2.970	1	11.491			
Benz[*c*]acridine	2.970	3	10.036	0.135	10.124	9.880
10-Methylbenz[*c*]acridine	2.970	1	10.668			
1,10-Dimethylbenz[*c*]acridine	2.970	1	10.945			
2,10-Dimethylbenz[*c*]acridine	2.970	1	11.490			
7,9-Dimethylbenz[*c*]acridine	2.970	1	11.457			
2,2'-Biquinoline	2.540	2	11.138	0.011	11.146	11.130
Pyrrole	0.613	1	2.865			

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
N-Methylpyrrole	0.559	1	2.923			
Pyrrolidine	0.406	2	2.893	0.014	2.903	2.883
N-Methylpyrrolidine	0.303	1	2.808			
Indole	1.200	8	5.505	0.161	5.675	5.209
N-Methylindole	1.206	2	5.765	0.305	5.980	5.549
2-Methylindole	1.200	3	6.180	0.019	6.197	6.160
3-Methylindole	1.200	5	6.114	0.060	6.170	6.024
5-Methylindole	1.200	3	6.121	0.080	6.212	6.067
7-Methylindole	1.200	2	6.081	0.047	6.114	6.048
2,N-Dimethylindole	1.206	1	6.362			
2,3-Dimethylindole	1.200	2	6.693	0.001	6.694	6.692
2,5-Dimethylindole	1.200	1	6.673			
2,7-Dimethylindole	1.200	1	6.459			
2,3,5-Trimethylindole	1.200	2	7.187	0.018	7.199	7.174
2,3,7-Trimethylindole	1.200	2	7.140	0.150	7.246	7.034
2-Phenylindole	1.810	5	8.966	0.168	9.187	8.819
Indoline	1.076	1	5.254			
5H-Indeno[1,2-*b*]pyridine	1.350	1	7.379			
Carbazole	1.787	9	7.982	0.093	8.149	7.836
1,2,3,4-Tetrahydrocarbazole	1.310	1	8.183			
1-Methylcarbazole	1.787	1	8.461			
2-Methylcarbazole	1.787	2	8.586	0.040	8.614	8.558
3-Methylcarbazole	1.787	1	8.590			
4-Methylcarbazole	1.787	1	8.681			
1,2-Dimethylcarbazole	1.787	1	9.137			
1,3-Dimethylcarbazole	1.787	1	9.170			
1,4-Dimethylcarbazole	1.787	1	9.014			
9-Ethylcarbazole	1.787	1	8.242			
9-Phenylcarbazole	2.400	2	10.033	0.069	10.082	9.984
Benzo[*a*]carbazole	2.400	2	10.556	0.024	10.573	10.539
Benzo[*b*]carbazole	2.400	2	10.788	0.042	10.818	10.758
Benzo[*c*]carbazole	2.400	1	10.824			
4-H-Benzo[*def*]carbazole	2.397	1	9.462			
Quinoxaline	1.304	1	5.654			
Pyrazole	0.620	1	3.151			
3-Methylpyrazole	0.586	1	3.672			
4-Methylpyrazole	0.586	1	3.674			
Imidazole	0.710	1	4.018			
N-Methylimidazole	0.589	1	3.805			
Pyrazine	0.629	1	2.920			
2-Methylpyrazine	0.629	1	3.254			
Chloropyrazine	0.727	1	3.867			
Pyrimidine	0.606	1	2.837			
Pyridazine	0.670	1	3.426			
3-Methylpyridazine	0.650	1	3.841			
Piperazine	0.570	1	3.400			
Thiophene	0.687	2	2.819	0.044	2.850	2.788
2-Methylthiophene	0.688	2	3.308	0.008	3.314	3.302
3-Methylthiophene	0.690	1	3.388			
2,5-Dimethylthiophene	0.690	2	3.769	0.053	3.806	3.731
2,3,5-Trimethylthiophene	0.690	1	4.511			

(Continued on p. 118)

TABLE I *(continued)*

Solute	R_2	No.	Average	S.D.	Max	Min
2,3,4,5-Tetramethylthiophene	0.690	1	5.158			
Benzo[*b*]thiophene	1.323	5	5.174	0.105	5.314	5.052
2-Methylbenzo[*b*]thiophene	1.323	2	5.610	0.016	5.621	5.598
3-Methylbenzo[*b*]thiophene	1.323	2	5.677	0.016	5.688	5.666
4-Methylbenzo[*b*]thiophene	1.323	1	5.692			
5-Methylbenzo[*b*]thiophene	1.323	1	5.661			
6-Methylbenzo[*b*]thiophene	1.323	1	5.661			
7-Methylbenzo[*b*]thiophene	1.323	1	5.574			
3,5-Dimethylbenzo[*b*]thiophene	1.323	1	6.295			
5-Ethylbenzo[*b*]thiophene	1.323	2	6.129	0.074	6.181	6.076
Dibenzothiophene	1.959	6	7.575	0.043	7.641	7.520
1,2,3,4-Tetrahydrodibenzothiophene	1.628	1	7.719			
trans-Hexahydrodibenzothiophene	1.300	1	7.113			
cis-Hexahydrodibenzothiophene	1.300	1	7.164			
1-Methyldibenzthiophene	1.959	1	8.316			
2-Methyldibenzothiophene	1.959	1	8.212			
3-Methyldibenzothiophene	1.959	1	8.216			
4-Methyldibenzothiophene	1.959	1	8.110			
1,7-Dimethyldibenzothiophene	1.959	1	8.897			
2,6-Dimethyldibenzothiophene	1.959	1	8.692			
2,8-Dimethyldibenzothiophene	1.959	1	8.794			
3,6-Dimethyldibenzothiophene	1.959	1	8.705			
3,7-Dimethyldibenzothiophene	1.959	1	8.798			
3,8-Dimethyldibenzothiophene	1.959	1	8.800			
4,6-Dimethyldibenzothiophene	1.959	1	8.596			
2-Ethyldibenzothiophene	1.959	1	8.698			
3-Ethyldibenzothiophene	1.959	1	8.571			
Benzo[*b*]naphtho[2,1-*d*]thiophene	2.570	2	10.162	0.021	10.177	10.147
2,[2'-Naphthyl)benzo[*b*]thiophene	2.660	2	11.317	0.035	11.342	11.292
Thianthrene	2.315	4	8.407	0.079	8.524	8.354

where $n(C)$ is number of carbon atoms in the alkyl group.

Once log L^{16} values were available, it then became possible to apply eqn. 2 or eqn. 5 to data sets, and then to calculate the π_2^H parameter, as described above. Again, data sets were restricted to those that included a reasonable number of solutes, around 15 as the minimum, and which led to regression equations of the required quality. For the determination of π_2^H values, the rations S.D./s or S.D./s' should now be as low as possible, and only equations where these ratios were less than or equal to 0.03 units were considered. Some 120 data sets were then left to be analyzed using eqn. 2 or eqn. 5. As for the log L^{16} values, once π_2^H values had been calculated, they were averaged and the entire process repeated. For a few regression equations a third round of calculations was carried out, but mostly this was not needed. A typical final regression equation is that for phenols on OV-1701 at 423 K [82],

$$I/10 = 2.991 - 22.683R_2 + 52.865\pi_2^H + 21.692\alpha_2^H + 20.579 \log L^{16} \quad (12)$$

$$n = 30 \quad \rho = 0.9987 \quad \text{S.D.} = 0.849$$

where S.D./s' = 0.016 units. Once again we could make little use of the very large data set of Peng *et al.* [94] on polar columns because of the very large S.D./I' value of 0.073 units, as shown in eqn. 13

TABLE II

SUBSTITUTENT VALUES FOR LOG L^{16} AND π_2^H IN PhX SOLUTES

Substituent X	$\Delta \log L^{16}$	$\Delta\pi_2^H$	μ (D)
H	0.000[a]	0.00[a]	0.00
Me	0.539[a]	0.00[a]	0.36
Et	0.992[a]	−0.01[a]	0.59
Pr	1.444[a]	−0.02[a]	0.35
Ph	3.228	0.47	0.00
F	0.002	0.05	1.66
Cl	0.871	0.13	1.75
Br	1.255	0.21	1.52
I	1.716	0.30	1.70
OMe	1.104	0.23	1.38
CHO	1.222	0.48	2.75
COMe	1.715	0.49	3.00
CO_2Me	1.918	0.33	1.80
CN	1.253	0.59	4.18
NH_2	1.148	0.44	1.57
NO_2	1.771	0.59	3.93
OH	0.980	0.37	1.55
SH	1.325	0.28	1.20
NHMe	1.692	0.38	1.67
NMe_2	1.915	0.32	1.57

[a] From ref. 5; log L^{16} for benzene is 2.786 and π_2^H for benzene is 0.52 units.

$$I/10 = 1.084 + 11.938R_2 + 57.217\pi_2^H + 94.986\alpha_2^H + 20.911 \log L^{16} \quad (13)$$

$n = 269 \quad \rho = 0.9956 \quad \text{S.D.} = 4.186$

The final calculated values of π_2^H for over 700 solutes are in Table III with the number of averaged values and the maximum and minimum values in the calculated π_2^H values. Also given are the α_2^H values that are needed to solve eqn. 2 or eqn. 5 for log π_2^H. Again, where π_2^H values are averages of three or more determinations, they can be regarded as reasonably firm values, but π_2^H values from a single determination must be only provisional. There are 52 π_2^H values in Table III that are averages of ten or more determinations; for these, S.D. values themselves average as 0.019 units. For the 41 π_2^H values that refer to functionally substituted aromatic compounds, as a subset, the average S.D. is 0.020 units. These error values agree well with the various S.D./s or S.D./s' values obtained in the regression equations, and so the estimated error in π_2^H can be set at 0.02 units.

Our estimated error in π_2^H, and in log L^{16} above, must be viewed in the light of the analysis of Poole *et al.* [99] who has shown that interfacial adsorption can make a significant contribution to the net retention of solutes. The effects of interfacial adsorption are particularly pronounced for less polar compounds such as alkanes on polar stationary phases at lower temperatures [99]. Since nearly all the data we have used, except for the excellent results of Poole and co-workers [86,87], is uncorrected for interfacial adsorption, it is necessary to consider possible errors from this source. First of all, most of the data we have used has been collected at temperatures of around 390 K or higher, where interfacial adsorption is not so pronounced. Secondly, we have concentrated on aromatic compounds, where again interfacial adsorption is much less significant than for aliphatic compounds. Finally, results in Table III may be compared with π_2^H values calculated only from the data of Poole and co-workers [86,87], see Table IV. It may be concluded that the present results are perfectly compatible with those derived from the corrected retention data of Poole and co-workers [86,87], and hence do not suffer from effects due to interfacial adsorption.

Estimation of π_2^H values

Before attempting any estimation of π_2^H values for multisubstituted benzenes, it is useful to dissect π_2^H values into contributions from dipolarity and polarisability. A plot of π_2^H for the monosubstituted benzenes in Table II against solute dipole moment is a quite scattered diagram, see Fig. 1, showing the dipole moment cannot make any very large contribution. An analysis of π_2^H values for all the chlorobenzenes (13, including benzene itself) is instructive, and a regression of π_2^H against the number of chlorine atoms in the solute, nCl, and the overall solute dipole moment, μ in D, yields eqn. 14,

$$\pi_2^H = 0.538 + 0.0743n\text{Cl} + 0.0353\mu \quad (14)$$

$n = 13 \quad \rho = 0.977 \quad \text{S.D.} = 0.030$

TABLE III

CALCULATED VALUES OF π_2^H

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
Cyclohexane	0.00	9	0.104	0.022	0.140	0.071	0.10
Methylcyclohexane	0.00	13	0.106	0.034	0.142	0.036	0.10
Cycloheptane	0.00	2	0.102	0.009	0.108	0.095	0.10
Cyclooctane	0.00	2	0.120	0.018	0.132	0.107	0.10
cis-Hydrindane	0.00	2	0.247	0.016	0.258	0.236	0.25
trans-Decalin	0.00	3	0.230	0.014	0.246	0.221	0.23
cis-Decalin	0.00	3	0.250	0.038	0.278	0.206	0.25
Cyclohexene	0.00	2	0.188	0.006	0.192	0.183	0.20
1-Methylcyclohexene	0.00	2	0.203	0.006	0.207	0.198	0.20
3-Methylcyclohexene	0.00	2	0.135	0.007	0.140	0.130	0.14
4-Methylcyclohexene	0.00	2	0.145	0.006	0.149	0.140	0.14
Cycloheptene	0.00	2	0.222	0.006	0.226	0.218	0.22
Cyclooctene	0.00	2	0.243	0.006	0.247	0.239	0.24
Cyclohexa-1,3-diene	0.00	3	0.302	0.015	0.318	0.289	0.30
Cyclohexa-1,4-diene	0.00	3	0.349	0.018	0.363	0.329	0.35
Cyclohepta-1,3-diene	0.00	3	0.381	0.007	0.387	0.374	0.38
Cycloocta-1,5-diene	0.00	2	0.359	0.005	0.362	0.355	0.36
Cyclohepta-1,3,5-triene	0.00	3	0.459	0.008	0.467	0.451	0.46
Cycloocta-1,3,5,7-tetraene	0.00	3	0.518	0.025	0.536	0.489	0.52
α-Pinene	0.00	1	0.185				0.20
Fluorocyclohexane	0.00	4	0.421	0.076	0.529	0.365	0.42
Chlorocyclohexane	0.00	5	0.478	0.028	0.519	0.455	0.48
Trichloroethene	0.00	1	0.367				0.37
Tetrachloroethene	0.00	1	0.442				0.44
1-Chlorocyclohexene	0.00	1	0.472				0.47
Bromocyclohexane	0.00	5	0.540	0.019	0.567	0.521	0.54
1-Bromocyclohexene	0.00	1	0.566				0.57
1-Bromo-4-methylcyclohexene	0.00	1	0.528				0.53
Iodocyclohexane	0.00	5	0.582	0.016	0.601	0.557	0.58
1-Iodocyclohexene	0.00	1	0.608				0.61
1,1-Difluorotetrachloroethane	0.00	1	0.334				0.33
1,2-Difluorotetrachloroethane	0.00	1	0.344				0.34
Methyl cyclohexyl ether	0.00	1	0.404				0.40
1,2-Dimethoxyethane	0.00	1	0.661				0.66
1,8-Cineole	0.00	1	0.497				0.50
Propenal	0.00	1	0.721				0.72
trans-But-2-ene-1-al	0.00	1	0.800				0.82
trans-Hex-2-ene-1-al	0.00	1	0.842				0.82
trans-Hept-2-ene-1-al	0.00	1	0.833				0.82
Carvone	0.00	1	0.934				0.93
Butan-2,3-dione	0.00	1	0.939				0.94
2-Methoxyethyl acetate	0.00	1	0.864				0.86
2-Ethoxyethyl acetate	0.00	2	0.819	0.041	0.848	0.790	0.82
Cyanocyclohexane	0.00	1	0.939	0.000	0.939	0.939	0.94
Cyclohexylamine	0.05	2	0.558	0.054	0.596	0.519	0.56
3-Methylcyclohexylamine	0.05	1	0.473				0.47
Nitrocyclohexane	0.00	1	0.971				0.97
Dimethylformamide	0.00	1	1.314				1.31
Dibutylformamide	0.00	1	1.114				1.11
Dimethylacetamide	0.00	1	1.332				1.33
2-Ethoxyethanol	0.30	1	0.501				0.50
trans-Hex-2-ene-1-ol	0.33	1	0.513				0.53

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
trans-Hept-2-ene-1-ol	0.33	1	0.538				0.53
trans-Oct-2-ene-1-ol	0.33	1	0.539				0.53
Dodecafluoroheptan-1-ol	0.65	1	0.500				0.50
Dimethylsulphoxide	0.00	1	1.744				1.74
Cyclopropylbenzene	0.00	1	0.647				0.65
Diphenylmethane	0.00	2	1.038	0.001	1.038	1.037	1.04
2-Methyldiphenylmethane	0.00	2	1.009	0.002	1.010	1.007	1.01
3-Methyldiphenylmethane	0.00	2	1.019	0.020	1.033	1.005	1.01
4-Methyldiphenylmethane	0.00	2	1.001	0.001	1.002	1.000	1.01
1,1-Diphenylethane	0.00	2	0.984	0.036	1.009	0.958	0.98
1,2-Diphenylethane	0.00	2	1.029	0.008	1.035	1.023	1.03
1,4-Diphenylbutane	0.00	2	1.045	0.013	1.054	1.036	1.04
Biphenyl	0.00	5	0.985	0.049	1.050	0.933	0.99
2-Methylbiphenyl	0.00	2	0.875	0.011	0.882	0.867	0.88
3-Methylbiphenyl	0.00	2	0.951	0.045	0.982	0.919	0.95
4-Methylbiphenyl	0.00	2	0.980	0.038	1.007	0.953	0.98
2-Ethylbiphenyl	0.00	2	0.828	0.011	0.835	0.820	0.83
3-Ethylbiphenyl	0.00	2	0.960	0.018	0.972	0.947	0.96
4-Ethylbiphenyl	0.00	2	0.962	0.026	0.980	0.943	0.96
2,3-Dimethylbiphenyl	0.00	2	0.890	0.020	0.904	0.876	0.89
2,4-Dimethylbiphenyl	0.00	2	0.858	0.015	0.868	0.847	0.86
2,5-Dimethylbiphenyl	0.00	2	0.855	0.018	0.867	0.842	0.86
2,6-Dimethylbiphenyl	0.00	2	0.767	0.037	0.793	0.741	0.77
3,4-Dimethylbiphenyl	0.00	2	0.988	0.035	1.012	0.963	0.99
3,5-Dimethylbiphenyl	0.00	2	0.950	0.013	0.959	0.940	0.95
2,2′-Dimethylbiphenyl	0.00	2	0.747	0.028	0.767	0.727	0.75
2,3′-Dimethylbiphenyl	0.00	2	0.864	0.032	0.886	0.841	0.86
2,4′-Dimethylbiphenyl	0.00	2	0.863	0.024	0.880	0.846	0.86
3,3′-Dimethylbiphenyl	0.00	2	0.931	0.035	0.955	0.906	0.93
3,4′-Dimethylbiphenyl	0.00	2	0.942	0.030	0.963	0.920	0.94
4,4′-Dimethylbiphenyl	0.00	2	0.960	0.028	0.979	0.940	0.96
2-Isopropylbiphenyl	0.00	2	0.823	0.062	0.867	0.779	0.82
3-Isopropylbiphenyl	0.00	2	0.906	0.003	0.908	0.904	0.91
4-Isopropylbiphenyl	0.00	2	0.930	0.005	0.933	0.926	0.93
o-Terphenyl	0.00	1	1.181				1.18
p-Terphenyl	0.00	1	1.483				1.48
trans-Stilbene	0.00	2	1.184	0.089	1.247	1.121	1.18
cis-Stilbene	0.00	2	0.982	0.013	0.991	0.972	0.98
α-Methylstilbene (*cis*, *trans*?)	0.00	2	1.065	0.009	1.071	1.058	1.06
1-Ethylnaphthalene	0.00	2	0.870	0.012	0.878	0.861	0.88
2-Ethylnaphthalene	0.00	2	0.904	0.011	0.912	0.896	0.90
1-*n*-Propylnaphthalene	0.00	1	0.880				0.88
2-*n*-Propylnaphthalene	0.00	1	0.870				0.87
2-Isopropylnaphthalene	0.00	1	0.865				0.86
1-*n*-Butylnaphthalene	0.00	1	0.882				0.88
2-*n*-Butylnaphthalene	0.00	1	0.874				0.87
1-Isobutylnaphthalene	0.00	1	0.851				0.85
2-Isobutylnaphthalene	0.00	1	0.848				0.85
2-*sec*.-Butylnaphthalene	0.00	1	0.842				0.84
2-*tert*.-Butylnaphthalene	0.00	1	0.842				0.84
1,3,7-Trimethylnaphthalene	0.00	1	0.919				0.91

(Continued on p. 122)

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
2,3,5-Trimethylnaphthalene	0.00	1	0.856				0.86
2,3,6-Trimethylnaphthalene	0.00	1	0.863				0.86
2-Phenylnaphthalene	0.00	1	1.198				1.20
2-Benzylnaphthalene	0.00	1	1.198				1.20
Acenaphthene	0.00	3	1.048	0.016	1.064	1.032	1.05
Acenaphthylene	0.00	2	1.141	0.009	1.147	1.134	1.14
Fluorene	0.00	3	1.059	0.084	1.122	0.963	1.06
9-Methylfluorene	0.00	1	1.487				1.50
Azulene	0.00	1	1.171				1.17
1-Methylazulene	0.00	1	0.965				0.97
5-Methylazulene	0.00	1	0.974				0.97
6-Methylazulene	0.00	1	0.979				0.97
4,6,8-Trimethylazulene	0.00	1	1.010				1.01
Anthracene	0.00	5	1.340	0.104	1.459	1.239	1.34
9,10-Dihydroanthracene	0.00	1	1.009				1.01
Phenanthrene	0.00	5	1.295	0.090	1.402	1.215	1.29
9,10-Dihydrophenanthrene	0.00	1	1.045				1.05
Fluoranthene	0.00	2	1.551	0.011	1.559	1.543	1.55
Benzo[*a*]fluorene	0.00	2	1.588	0.009	1.594	1.581	1.59
Benzo[*b*]fluorene	0.00	2	1.565	0.010	1.572	1.558	1.57
3,4-Benzfluorene	0.00	1	1.586				1.59
Pyrene	0.00	3	1.716	0.030	1.744	1.684	1.72
Benz[*a*]anthracene	0.00	2	1.699	0.011	1.707	1.691	1.70
Benz[*c*]phenanthrene	0.00	1	1.683				1.68
Chrysene	0.00	2	1.729	0.006	1.733	1.725	1.73
Triphenylene	0.00	2	1.713	0.007	1.718	1.708	1.71
Benz[*b*]fluoranthene	0.00	1	1.824				1.82
Benz[*j*]fluoranthene	0.00	1	1.909				1.91
Benz[*k*]fluoranthene	0.00	1	1.912				1.91
Benz[*ghi*]fluoranthene	0.00	1	1.834				1.83
Perylene	0.00	2	1.794	0.016	1.805	1.783	1.79
3-Methylcholanthrene	0.00	1	1.570				1.57
Dibenz[*ac*]anthracene	0.00	2	1.927	0.008	1.933	1.921	1.93
Dibenz[*ah*]anthracene	0.00	1	2.044				2.04
Benz[*a*]pyrene	0.00	2	1.980	0.028	2.000	1.960	1.98
3,4-Benzpyrene	0.00	1	1.917				1.92
Benz[*e*]pyrene	0.00	1	1.994				1.99
Benz[*b*]chrysene	0.00	1	2.189				2.19
Pentacene	0.00	1	2.714				2.71
Benz[*ghi*]perylene	0.00	2	1.897	0.013	1.906	1.887	1.90
Picene	0.00	2	2.041	0.035	2.066	2.016	2.04
Fluorobenzene	0.00	32	0.571	0.016	0.617	0.536	0.57
1,2-Difluorobenzene	0.00	2	0.755	0.000	0.755	0.755	0.75
1,2,4,5-Tetrafluorobenzene	0.00	3	0.697	0.067	0.740	0.620	0.70
Pentafluorobenzene	0.00	3	0.680	0.113	0.750	0.550	0.68
Hexafluorobenzene	0.00	3	0.657	0.167	0.790	0.470	0.66
2-Fluorotoluene	0.00	4	0.572	0.027	0.600	0.536	0.57
3-Fluorotoluene	0.00	4	0.585	0.032	0.610	0.539	0.58
4-Fluorotoluene	0.00	5	0.548	0.038	0.590	0.493	0.55
Benzotrifluoride	0.00	16	0.485	0.026	0.540	0.438	0.48
Chlorobenzene	0.00	36	0.655	0.015	0.687	0.618	0.65
1,2-Dichlorobenzene	0.00	18	0.779	0.022	0.812	0.725	0.78
1,3-Dichlorobenzene	0.00	17	0.727	0.019	0.752	0.686	0.73

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
1,4-Dichlorobenzene	0.00	17	0.752	0.021	0.771	0.698	0.75
1,2,3-Trichlorobenzene	0.00	5	0.858	0.019	0.888	0.840	0.86
1,2,4-Trichlorobenzene	0.00	5	0.810	0.031	0.856	0.771	0.81
1,3,5-Trichlorobenzene	0.00	5	0.728	0.053	0.795	0.653	0.73
1,2,3,4-Tetrachlorobenzene	0.00	4	0.919	0.012	0.933	0.904	0.92
1,2,3,5-Tetrachlorobenzene	0.00	5	0.845	0.042	0.894	0.780	0.85
1,2,4,5-Tetrachlorobenzene	0.00	5	0.859	0.033	0.899	0.808	0.86
Pentachlorobenzene	0.00	4	0.957	0.014	0.976	0.947	0.96
Hexachlorobenzene	0.00	4	0.990	0.015	1.006	0.971	0.99
2-Chlorotoluene	0.00	13	0.650	0.010	0.664	0.629	0.65
3-Chlorotoluene	0.00	14	0.672	0.014	0.703	0.646	0.67
4-Chlorotoluene	0.00	14	0.669	0.019	0.704	0.638	0.67
2,4-Dichlorotoluene	0.00	5	0.742	0.030	0.784	0.706	0.74
2,5-Dichlorotoluene	0.00	3	0.757	0.011	0.767	0.745	0.76
2,6-Dichlorotoluene	0.00	5	0.750	0.030	0.789	0.715	0.75
3,4-Dichlorotoluene	0.00	3	0.803	0.025	0.831	0.786	0.80
2,3,4-Trichlorotoluene	0.00	2	0.874	0.001	0.874	0.873	0.87
2,3,5-Trichlorotoluene	0.00	2	0.844	0.008	0.849	0.838	0.84
2,4,5-Trichlorotoluene	0.00	2	0.855	0.026	0.873	0.836	0.85
2,4,6-Trichlorotoluene	0.00	2	0.772	0.002	0.773	0.770	0.77
2,3,4,5-Tetrachlorotoluene	0.00	2	0.943	0.006	0.947	0.938	0.94
2,3,5,6-Tetrachlorotuluene	0.00	2	0.914	0.026	0.932	0.895	0.91
Pentachlorotoluene	0.00	2	0.996	0.052	1.033	0.959	1.00
2-Chloro-*p*-xylene	0.00	4	0.706	0.068	0.807	0.665	0.71
2,3-Dichloro-*p*-xylene	0.00	3	0.816	0.020	0.827	0.793	0.82
2,5-Dichloro-*p*-xylene	0.00	3	0.779	0.012	0.790	0.767	0.78
2,3,5-Trichloro-*p*-xylene	0.00	3	0.867	0.011	0.880	0.861	0.87
Benzyl chloride	0.00	6	0.818	0.062	0.879	0.731	0.82
2-Chlorobenzyl chloride	0.00	2	0.983	0.008	0.988	0.977	0.98
4-Chlorobenzyl chloride	0.00	3	0.879	0.020	0.892	0.856	0.88
2-Chloro-4-methylbenzyl chloride	0.00	1	1.038				1.03
3-Chloro-4-methylbenzyl chloride	0.00	1	1.067				1.06
1,4-Bis(chloromethyl)benzene	0.00	1	1.338				1.34
Benzal chloride	0.10	3	0.788	0.019	0.806	0.769	0.79
Benzotrichloride	0.00	1	0.843				0.84
2-Chlorostyrene	0.00	2	0.669	0.018	0.681	0.656	0.67
Bromobenzene	0.00	30	0.732	0.016	0.766	0.691	0.73
1,2-Dibromobenzene	0.00	2	0.960	0.003	0.962	0.958	0.96
1,3-Dibromobenzene	0.00	2	0.878	0.004	0.880	0.875	0.88
1,4-Dibromobenzene	0.00	1	0.861	0.000	0.861	0.861	0.86
2-Bromotoluene	0.00	3	0.723	0.003	0.725	0.720	0.72
3-Bromotoluene	0.00	4	0.746	0.005	0.752	0.741	0.75
4-Bromotoluene	0.00	4	0.737	0.006	0.744	0.732	0.74
Benzyl bromide	0.00	1	0.978				0.98
2-Bromo-1-phenylethane	0.00	1	0.937				0.94
1-Bromonaphthalene	0.00	1	1.037				1.04
Iodobenzene	0.00	29	0.823	0.024	0.878	0.764	0.82
1,2-Diiodobenzene	0.00	2	1.208	0.004	1.210	1.205	1.21
1,3-Diiodobenzene	0.00	2	1.071	0.004	1.074	1.068	1.07
1,4-Diiodobenzene	0.00	2	1.150	0.004	1.153	1.147	1.15
2-Iodotoluene	0.00	3	0.822	0.021	0.846	0.807	0.82

(Continued on p. 124)

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
3-Iodotoluene	0.00	3	0.838	0.022	0.863	0.823	0.84
4-Iodotoluene	0.00	1	0.850				0.85
Methylphenylether	0.00	30	0.745	0.026	0.778	0.659	0.75
2-Methylanisole	0.00	3	0.745	0.003	0.748	0.742	0.75
3-Methylanisole	0.00	3	0.779	0.006	0.784	0.772	0.78
4-Methylanisole	0.00	3	0.773	0.002	0.776	0.772	0.77
2,3-Dimethylanisole	0.00	2	0.793	0.001	0.794	0.792	0.79
2,4-Dimethylanisole	0.00	2	0.774	0.014	0.784	0.764	0.77
2,5-Dimethylanisole	0.00	2	0.795	0.016	0.806	0.784	0.79
2,6-Dimethylanisole	0.00	2	0.781	0.012	0.789	0.772	0.78
3,4-Dimethylanisole	0.00	2	0.807	0.010	0.814	0.800	0.81
3,5-Dimethylanisole	0.00	2	0.783	0.029	0.803	0.762	0.78
2-Ethylanisole	0.00	2	0.796	0.006	0.800	0.792	0.80
3-Ethylanisole	0.00	2	0.813	0.004	0.816	0.810	0.80
4-Ethylanisole	0.00	2	0.798	0.006	0.802	0.794	0.80
2-Propylanisole	0.00	2	0.806	0.014	0.816	0.796	0.80
3-Propylanisole	0.00	2	0.813	0.001	0.814	0.812	0.80
4-Propylanisole	0.00	2	0.797	0.004	0.800	0.794	0.80
4-Allylanisole	0.00	2	0.830	0.017	0.842	0.818	0.83
2-Fluoroanisole	0.00	4	0.790	0.042	0.836	0.744	0.79
3-Fluoroanisole	0.00	4	0.718	0.033	0.760	0.682	0.72
4-Fluoroanisole	0.00	6	0.735	0.035	0.772	0.680	0.74
2-Chloroanisole	0.00	3	0.915	0.018	0.936	0.904	0.91
3-Chloroanisole	0.00	1	0.860				0.86
4-Chloroanisole	0.00	5	0.862	0.023	0.890	0.832	0.86
2,3-Dichloroanisole	0.00	1	1.021				1.02
2,4-Dichloroanisole	0.00	3	0.943	0.025	0.960	0.915	0.94
2,5-Dichloroanisole	0.00	3	0.950	0.010	0.959	0.939	0.95
2,6-Dichloroanisole	0.00	3	0.863	0.012	0.870	0.850	0.86
3,4-Dichloroanisole	0.00	1	0.946				0.95
3,5-Dichloroanisole	0.00	1	0.868				0.87
2,3,4-Trichloroanisole	0.00	1	1.118				1.12
2,3,5-Trichloroanisole	0.00	1	1.007				1.01
2,3,6-Trichloroanisole	0.00	1	0.906				0.91
2,4,5-Trichloroanisole	0.00	3	1.006	0.014	1.021	0.993	1.01
2,4,6-Trichloroanisole	0.00	3	0.846	0.034	0.884	0.818	0.85
3,4,5-Trichloroanisole	0.00	1	0.988				0.99
2,3,4,5-Tetrachloroanisole	0.00	1	1.146				1.15
2,3,4,6-Tetrachloroanisole	0.00	3	0.953	0.033	0.983	0.917	0.95
2,3,5,6-Tetrachloroanisole	0.00	1	0.915				0.92
Pentachloroanisole	0.00	3	1.055	0.051	1.099	0.999	1.05
4-Bromoanisole	0.00	2	0.902	0.008	0.907	0.896	0.90
4-Iodoanisole	0.00	2	0.991	0.021	1.005	0.976	0.99
Methyl benzyl ether	0.00	1	0.771				0.77
Ethyl benzyl ether	0.00	1	0.710				0.71
Diphenyl ether	0.00	2	1.084	0.089	1.147	1.021	1.08
1,2-Dimethoxybenzene	0.00	2	0.965	0.070	1.014	0.915	0.97
1,3-Dimethoxybenzene	0.00	1	1.011				1.01
4-Methylveratrole	0.00	2	0.949	0.001	0.950	0.948	0.95
3-Chloroveratrole	0.00	1	0.959				0.96
4-Chloroveratrole	0.00	1	1.027				1.03
3,4-Dichloroveratrole	0.00	1	1.051				1.05
3,5-Dichloroveratrole	0.00	1	0.979				0.98

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
3,6-Dichloroveratrole	0.00	1	0.895				0.90
4,5-Dichloroveratrole	0.00	1	1.114				1.11
3,4,5-Trichloroveratrole	0.00	1	1.102				1.10
3,4,6-Trichloroveratrole	0.00	1	0.925				0.93
Tetrachloroveratrole	0.00	1	1.004				1.00
Benzaldehyde	0.00	22	0.999	0.013	1.020	0.967	1.00
2-Methylbenzaldehyde	0.00	2	0.959	0.010	0.966	0.952	0.96
3-Methylbenzaldehyde	0.00	2	0.973	0.018	0.986	0.960	0.97
4-Methylbenzaldehyde	0.00	2	1.004	0.020	1.018	0.990	1.00
2,4-Dimethylbenzaldehyde	0.00	2	0.932	0.001	0.932	0.931	0.93
2,5-Dimethylbenzaldehyde	0.00	2	0.927	0.012	0.935	0.918	0.93
3,4-Dimethylbenzaldehyde	0.00	2	0.923	0.025	0.940	0.905	0.92
4-Isopropylbenzaldehyde	0.00	2	0.968	0.001	0.968	0.967	0.97
Furfural	0.00	1	1.134				1.13
Phthalaldehyde	0.00	2	1.291	0.052	1.327	1.254	1.29
Terephthalaldehyde	0.00	2	1.294	0.059	1.335	1.252	1.29
Acetophenone	0.00	18	1.007	0.023	1.074	0.978	1.01
2-Methoxyacetophenone	0.00	2	0.993	0.001	0.994	0.992	0.99
3-Methoxyacetophenone	0.00	2	0.970	0.006	0.974	0.966	0.97
4-Methoxyacetophenone	0.00	2	0.971	0.010	0.978	0.964	0.97
4-Phenylbutan-2-one	0.00	1	1.144				1.14
Methyl benzoate	0.00	23	0.851	0.032	0.939	0.779	0.85
Ethyl benzoate	0.00	2	0.854	0.006	0.858	0.850	0.85
Propyl benzoate	0.00	1	0.794				0.80
Butyl benzoate	0.00	1	0.797				0.80
Pentyl benzoate	0.00	1	0.786				0.79
Hexyl benzoate	0.00	1	0.787				0.79
Heptyl benzoate	0.00	1	0.788				0.79
Octyl benzoate	0.00	1	0.786				0.79
Nonyl benzoate	0.00	1	0.784				0.78
Decyl benzoate	0.00	1	0.783				0.78
Undecyl benzoate	0.00	1	0.784				0.78
Dodecyl benzoate	0.00	1	0.782				0.78
Methyl 2-methylbenzoate	0.00	3	0.866	0.054	0.926	0.821	0.87
Methyl 3-methylbenzoate	0.00	3	0.878	0.048	0.929	0.833	0.88
Methyl 4-methylbenzoate	0.00	3	0.881	0.045	0.930	0.842	0.88
Methyl 2,4-dimethylbenzoate	0.00	2	0.760	0.052	0.797	0.723	0.80
Methyl 2,5-dimethylbenzoate	0.00	2	0.776	0.040	0.804	0.747	0.80
Methyl 3,4-dimethylbenzoate	0.00	2	0.854	0.040	0.882	0.825	0.85
Methyl 4-isopropylbenzoate	0.00	2	0.785	0.024	0.802	0.768	0.80
Methyl 2-fluorobenzoate	0.00	4	0.888	0.042	0.928	0.832	0.89
Methyl 3-fluorobenzoate	0.00	4	0.883	0.071	0.974	0.816	0.88
Methyl 4-fluorobenzoate	0.00	4	0.885	0.070	0.971	0.819	0.89
Methyl 2-chlorobenzoate	0.00	3	0.989	0.024	1.015	0.968	0.99
Methyl 4-chlorobenzoate	0.00	1	0.917				0.92
Methyl 2,4-dichlorobenzoate	0.00	2	0.976	0.026	0.994	0.957	0.98
Methyl 2,5-dichlorobenzoate	0.00	2	0.986	0.027	1.005	0.967	0.99
Methyl 2,3,6-trichlorobenzoate	0.00	2	1.077	0.020	1.091	1.063	1.08
Methyl 2-MeO-3,6-dichlorobenzoate	0.00	2	1.038	0.019	1.051	1.024	1.04
Methyl 4-methoxybenzoate	0.00	1	1.313				1.31
Phenyl acetate	0.00	1	1.131				1.13

(Continued on p. 126)

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
2-Methylphenyl acetate	0.00	1	1.039				1.04
3-Methylphenyl acetate	0.00	1	1.132				1.13
4-Methylphenyl acetate	0.00	3	1.006	0.121	1.144	0.920	1.01
Benzyl acetate	0.00	2	1.065	0.050	1.100	1.029	1.06
2-Methylbenzyl acetate	0.00	2	0.957	0.013	0.966	0.947	0.96
4-Methylbenzyl acetate	0.00	2	1.003	0.024	1.020	0.986	1.00
2,4-Dimethylbenzyl acetate	0.00	2	0.913	0.025	0.931	0.895	0.91
2,5-Dimethylbenzyl acetate	0.00	2	0.914	0.018	0.926	0.901	0.91
3,4-Dimethylbenzyl acetate	0.00	2	0.909	0.042	0.939	0.879	0.91
2-Phenylethyl acetate	0.00	1	1.096				1.10
Benzyl benzoate	0.00	2	1.355	0.136	1.451	1.258	1.35
Methyl phenylacetate	0.00	1	1.134				1.13
Ethyl phenylacetate	0.00	1	1.008				1.01
Ethyl cinnamate	0.00	1	1.237				1.24
Dimethyl phthalate	0.00	2	1.407	0.035	1.432	1.382	1.41
Dimethyl isophthalate	0.00	2	1.256	0.027	1.275	1.237	1.26
Dimethyl terephthalate	0.00	2	1.219	0.025	1.236	1.201	1.22
Dimethyl methylterephthalate	0.00	2	1.172	0.006	1.176	1.167	1.17
Benzonitrile	0.00	21	1.110	0.019	1.157	1.078	1.11
2-Methylbenzonitrile	0.00	2	1.056	0.015	1.066	1.045	1.06
3-Methylbenzonitrile	0.00	1	1.075				1.08
4-Methylbenzonitrile	0.00	1	1.097				1.10
2-Chlorobenzonitrile	0.00	1	1.236				1.24
3-Chlorobenzonitrile	0.00	1	1.139				1.14
4-Chlorobenzonitrile	0.00	1	1.180				1.18
4-Nitrobenzonitrile	0.00	1	1.331				1.33
Phenylacetonitrile	0.00	1	1.152				1.15
Aniline	0.26	29	0.960	0.023	1.005	0.907	0.96
o-Toluidine	0.23	9	0.923	0.022	0.955	0.880	0.92
m-Toluidine	0.23	10	0.950	0.018	0.978	0.928	0.95
p-Toluidine	0.23	11	0.948	0.027	0.987	0.902	0.95
2-Ethylaniline	0.23	3	0.853	0.021	0.875	0.834	0.85
3-Ethylaniline	0.23	2	0.946	0.006	0.950	0.942	0.95
4-Ethylaniline	0.23	4	0.910	0.034	0.959	0.885	0.91
2,3-Dimethylaniline	0.20	5	0.962	0.024	0.981	0.922	0.96
2,4-Dimethylaniline	0.20	5	0.951	0.006	0.958	0.945	0.95
2,5-Dimethylaniline	0.20	4	0.931	0.023	0.964	0.912	0.93
2,6-Dimethylaniline	0.20	7	0.891	0.018	0.912	0.860	0.89
3,4-Dimethylaniline	0.20	6	0.971	0.020	0.995	0.954	0.97
3,5-Dimethylaniline	0.20	2	0.949	0.004	0.952	0.946	0.95
2,6-Diethylaniline	0.20	1	0.556				0.56
2-Vinylaniline	0.25	1	0.984				0.98
3-Vinylaniline	0.26	1	1.120				1.12
4-Vinylaniline	0.25	1	1.100				1.10
2-Fluoroaniline	0.28	3	0.879	0.024	0.907	0.864	0.88
3-Fluoroaniline	0.30	5	1.075	0.081	1.185	0.979	1.08
4-Fluoroaniline	0.28	8	1.095	0.073	1.175	1.004	1.09
2-Chloroaniline	0.30	6	0.923	0.016	0.940	0.903	0.92
3-Chloroaniline	0.33	7	1.099	0.041	1.146	1.050	1.10
4-Chloroaniline	0.30	5	1.127	0.040	1.167	1.073	1.13
2-Bromoaniline	0.31	5	0.979	0.025	1.001	0.942	0.98
3-Bromoaniline	0.33	6	1.186	0.028	1.215	1.155	1.19
4-Bromoaniline	0.31	6	1.189	0.035	1.229	1.145	1.19

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
2-Iodoaniline	0.31	1	1.000				1.00
3-Iodoaniline	0.33	5	1.258	0.025	1.282	1.229	1.26
4-Iodoaniline	0.31	3	1.278	0.014	1.294	1.266	1.28
2-Cyanoaniline	0.35	1	1.374				1.37
3-Cyanoaniline	0.38	1	1.594				1.59
4-Cyanoaniline	0.40	1	1.779				1.78
2-Methoxyaniline	0.23	5	1.027	0.051	1.083	0.982	1.00
3-Methoxyaniline	0.25	6	1.216	0.026	1.241	1.168	1.22
4-Methoxyaniline	0.23	5	1.194	0.039	1.231	1.148	1.10
2-Nitroaniline	0.37	2	1.365	0.034	1.389	1.341	1.36
3-Nitroaniline	0.40	3	1.713	0.102	1.823	1.623	1.71
4-Nitroaniline	0.42	3	1.906	0.019	1.928	1.895	1.91
2-Ethoxyaniline	0.23	1	1.111				1.10
3-Ethoxyaniline	0.25	1	1.090				1.10
4-Ethoxyaniline	0.23	3	1.173	0.084	1.224	1.076	1.17
3-Fluoro-4-methylaniline	0.27	2	1.160	0.001	1.161	1.159	1.16
4-Fluoro-2-methylaniline	0.25	2	1.140	0.001	1.141	1.139	1.14
2,4-Difluoroaniline	0.30	2	1.021	0.001	1.021	1.020	1.02
2,5-Difluoroaniline	0.32	2	1.149	0.001	1.150	1.148	1.15
N-Methylaniline	0.17	10	0.898	0.020	0.934	0.881	0.90
N-Ethylaniline	0.17	5	0.851	0.042	0.887	0.784	0.85
N-Propylaniline	0.17	4	0.853	0.014	0.867	0.840	0.85
N-Butylaniline	0.17	4	0.855	0.006	0.860	0.847	0.85
N-Isopentylaniline	0.17	2	0.845	0.002	0.846	0.843	0.84
2-Methyl-N-methylaniline	0.17	2	0.977	0.000	0.977	0.977	0.98
3-Methyl-N-methylaniline	0.17	2	1.004	0.001	1.004	1.003	1.00
4-Methyl-N-methylaniline	0.17	2	0.977	0.040	1.005	0.949	0.98
2-Methyl-N-ethylaniline	0.17	4	0.842	0.038	0.878	0.807	0.84
3-Methyl-N-ethylaniline	0.17	4	0.898	0.014	0.912	0.885	0.90
4-Methyl-N-ethylaniline	0.17	4	0.886	0.023	0.907	0.865	0.90
2-Chloro-N-methylaniline	0.19	2	0.961	0.002	0.962	0.959	0.96
4-Chloro-N-methylaniline	0.21	2	1.011	0.001	1.011	1.010	1.01
N,N-Dimethylaniline	0.00	11	0.842	0.016	0.869	0.817	0.84
N,N-Diethylaniline	0.00	7	0.799	0.026	0.834	0.772	0.80
2-Methyl-N,N-dimethylaniline	0.00	5	0.651	0.051	0.740	0.620	0.65
3-Methyl-N,N-dimethylaniline	0.00	5	0.861	0.016	0.889	0.851	0.86
4-Methyl-N,N-dimethylaniline	0.00	6	0.827	0.015	0.849	0.811	0.83
4-Bromo-N,N-dimethylaniline	0.00	4	0.968	0.050	1.012	0.924	0.97
3-Methyl-N,N-diethylaniline	0.00	4	0.793	0.032	0.822	0.764	0.79
4-Methyl-N,N-diethylaniline	0.00	4	0.797	0.040	0.833	0.761	0.80
1-Naphthylamine	0.20	2	1.257	0.001	1.258	1.256	1.26
2-Naphthylamine	0.22	2	1.276	0.000	1.276	1.276	1.28
Benzylamine	0.10	2	0.879	0.058	0.920	0.838	0.88
Nitrobenzene	0.00	20	1.108	0.019	1.153	1.064	1.11
2-Nitrotoluene	0.00	2	1.114	0.021	1.129	1.099	1.11
3-Nitrotoluene	0.00	2	1.101	0.011	1.108	1.093	1.10
4-Nitrotoluene	0.00	1	1.114				1.11
1-Fluoro-3-nitrobenzene	0.00	4	1.108	0.172	1.330	0.930	1.11
1-Chloro-2-nitrobenzene	0.00	3	1.253	0.005	1.256	1.248	1.25
1-Chloro-3-nitrobenzene	0.00	3	1.133	0.032	1.169	1.108	1.13
1-Chloro-4-nitrobenzene	0.00	3	1.168	0.020	1.184	1.145	1.17

(Continued on p. 128)

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
1-Methoxy-4-nitrobenzene	0.00	1	1.213				1.21
Phenol	0.60	46	0.892	0.020	0.942	0.839	0.89
o-Cresol	0.52	32	0.862	0.018	0.895	0.821	0.86
m-Cresol	0.57	33	0.879	0.014	0.902	0.847	0.88
p-Cresol	0.57	33	0.873	0.016	0.906	0.843	0.87
2-Ethylphenol	0.52	11	0.841	0.039	0.919	0.776	0.84
3-Ethylphenol	0.55	16	0.906	0.017	0.930	0.871	0.91
4-Ethylphenol	0.55	16	0.899	0.020	0.935	0.867	0.90
2,3-Dimethylphenol	0.53	23	0.808	0.022	0.870	0.763	0.81
2,4-Dimethylphenol	0.53	24	0.797	0.013	0.830	0.770	0.80
2,5-Dimethylphenol	0.54	18	0.789	0.012	0.807	0.761	0.79
2,6-Dimethylphenol	0.86	22	0.787	0.031	0.846	0.702	0.79
3,4-Dimethylphenol	0.56	19	0.865	0.031	0.947	0.818	0.86
3,5-Dimethylphenol	0.57	23	0.840	0.020	0.872	0.792	0.84
2-*n*-Propylphenol	0.52	6	0.859	0.019	0.888	0.833	0.86
3-*n*-Propylphenol	0.55	5	0.896	0.020	0.913	0.864	0.90
4-*n*-Propylphenol	0.55	6	0.875	0.014	0.895	0.864	0.88
2-Isopropylphenol	0.52	7	0.885	0.051	0.985	0.834	0.89
3-Isopropylphenol	0.55	7	0.917	0.024	0.971	0.905	0.92
4-Isopropylphenol	0.55	7	0.894	0.027	0.952	0.872	0.89
2-Methyl-4-ethylphenol	0.53	4	0.787	0.015	0.805	0.774	0.79
2-Methyl-5-ethylphenol	0.54	3	0.782	0.009	0.791	0.773	0.78
3-Methyl-4-ethylphenol	0.56	2	0.886	0.030	0.907	0.864	0.89
3-Methyl-5-ethylphenol	0.57	4	0.854	0.020	0.880	0.834	0.85
3-Methyl-6-ethylphenol	0.54	3	0.870	0.053	0.931	0.834	0.87
4-Methyl-2-ethylphenol	0.53	4	0.789	0.040	0.818	0.730	0.79
2,3,4-Trimethylphenol	0.52	3	0.821	0.025	0.849	0.800	0.82
2,3,5-Trimethylphenol	0.52	12	0.840	0.012	0.852	0.819	0.84
2,3,6-Trimethylphenol	0.37	7	0.808	0.046	0.864	0.719	0.81
2,4,5-Trimethylphenol	0.52	3	0.791	0.027	0.817	0.764	0.79
2,4,6-Trimethylphenol	0.37	11	0.791	0.033	0.824	0.724	0.78
3,4,5-Trimethylphenol	0.55	6	0.881	0.027	0.920	0.842	0.88
2-*n*-Butylphenol	0.52	4	0.839	0.019	0.855	0.812	0.84
3-*n*-Butylphenol	0.55	4	0.909	0.028	0.924	0.867	0.91
4-*n*-Butylphenol	0.55	4	0.879	0.007	0.886	0.870	0.88
2-*sec.*-Butylphenol	0.52	5	0.905	0.032	0.947	0.868	0.91
4-*sec.*-Butylphenol	0.55	5	0.907	0.007	0.916	0.899	0.91
2-*tert.*-Butylphenol	0.52	7	0.924	0.034	0.977	0.886	0.92
4-*tert.*-Butylphenol	0.56	7	0.888	0.010	0.906	0.876	0.89
2,4-Diethylphenol	0.53	3	0.833	0.022	0.858	0.817	0.83
2,5-Diethylphenol	0.54	2	0.857	0.033	0.880	0.834	0.86
2,6-Diethylphenol	0.39	1	0.847				0.85
2-Methyl-6-propylphenol	0.39	3	0.703	0.024	0.725	0.677	0.70
4-Methyl-2-propylphenol	0.53	3	0.796	0.017	0.812	0.779	0.80
2-Methyl-4-isopropylphenol	0.53	1	0.844				0.84
3-Methyl-5-isopropylphenol	0.57	1	0.736				0.74
3,4-Dimethyl-6-ethylphenol	0.52	1	0.794				0.79
2,3,4,5-Tetramethylphenol	0.52	3	0.873	0.058	0.940	0.835	0.87
2,3,5,6-Tetramethylphenol	0.35	7	0.860	0.028	0.885	0.807	0.86
2-Ethyl-5-propylphenol	0.54	3	0.829	0.025	0.856	0.807	0.83
Pentamethylphenol	0.35	4	0.852	0.028	0.879	0.816	0.85
2,6-Diisopropylphenol	0.38	2	0.750	0.059	0.791	0.708	0.75
4-Methyl-2,6-di-*tert.*-butylphenol	0.37	2	0.706	0.042	0.735	0.676	0.71

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
Thymol	0.52	6	0.791	0.031	0.850	0.763	0.79
Carvacrol	0.54	4	0.814	0.033	0.860	0.789	0.81
4-*tert.*-Pentylphenol	0.56	4	0.885	0.012	0.903	0.874	0.89
2-Phenylphenol	0.56	1	1.030				1.03
4-Phenylphenol	0.59	1	1.482				1.48
5,6,7,8-Tetrahydro-1-naphthol	0.53	3	0.715	0.019	0.728	0.693	0.72
5,6,7,8-Tetrahydro-2-naphthol	0.56	2	0.758	0.006	0.762	0.754	0.76
4-Indanol	0.53	5	0.802	0.019	0.823	0.778	0.80
5-Indanol	0.56	5	0.834	0.016	0.855	0.813	0.83
5-Methyl-4-indanol	0.37	2	0.803	0.093	0.869	0.737	0.80
6-Methyl-4-indanol	0.52	3	0.778	0.005	0.784	0.774	0.78
7-Methyl-4-indanol	0.52	3	0.791	0.010	0.803	0.784	0.79
7-Methyl-5-indanol	0.55	2	0.839	0.006	0.843	0.834	0.84
2-Fluorophenol	0.61	3	0.687	0.004	0.691	0.684	0.69
3-Fluorophenol	0.68	3	0.976	0.012	0.990	0.967	0.98
4-Fluorophenol	0.63	7	0.954	0.053	1.014	0.861	0.95
2-Chlorophenol	0.32	3	0.884	0.026	0.913	0.854	0.86
3-Chlorophenol	0.69	11	1.058	0.014	1.075	1.040	1.06
4-Chlorophenol	0.67	12	1.076	0.011	1.105	1.064	1.08
2-Bromophenol	0.35	1	0.901				0.55
3-Bromophenol	0.70	7	1.153	0.031	1.200	1.112	1.15
4-Bromophenol	0.67	7	1.169	0.015	1.198	1.156	1.17
2-Iodophenol	0.40	1	1.000				0.65
3-Iodophenol	0.70	1	1.204				1.20
4-Iodophenol	0.68	4	1.332	0.108	1.486	1.250	1.33
3,4-Dichlorophenol	0.74	2	1.202	0.076	1.256	1.148	1.20
3,5-Dichlorophenol	0.77	4	1.166	0.031	1.210	1.143	1.17
3,4,5-Trichlorophenol	0.82	2	1.465	0.057	1.505	1.425	1.46
4-Chloro-2-methylphenol	0.63	1	0.907				0.91
4-Chloro-3-methylphenol	0.65	4	1.022	0.044	1.067	0.964	1.02
2-Methoxyphenol	0.26	9	0.910	0.039	0.950	0.852	0.91
3-Methoxyphenol	0.59	7	1.174	0.025	1.196	1.124	1.17
4-Methoxyphenol	0.57	9	1.170	0.011	1.193	1.153	1.17
2,6-Dimethoxyphenol	0.25	2	0.900	0.057	0.940	0.860	0.90
4-Allyl-2-methoxyphenol	0.26	3	0.796	0.035	0.819	0.756	0.80
4-Propyl-2-methoxyphenol	0.26	3	0.755	0.020	0.773	0.733	0.76
2-Cyanophenol	0.74	2	1.328	0.049	1.363	1.293	1.33
3-Cyanophenol	0.77	3	1.548	0.014	1.559	1.533	1.55
4-Cyanophenol	0.79	3	1.626	0.014	1.642	1.614	1.63
2-Nitrophenol	0.05	5	1.048	0.080	1.093	0.907	0.82
3-Nitrophenol	0.79	5	1.569	0.007	1.576	1.560	1.57
4-Nitrophenol	0.82	5	1.720	0.029	1.759	1.693	1.72
3-Methyl-2-nitrophenol	0.05	1	1.082				1.08
2-Methyl-4-nitrophenol	0.78	1	1.614				1.61
2-Methyl-5-nitrophenol	0.75	1	1.520				1.52
2-Methyl-6-nitrophenol	0.05	1	1.064				1.06
2,5-Dimethyl-4-nitrophenol	0.79	1	1.551				1.55
2,6-Dimethyl-4-nitrophenol	0.79	1	1.536				1.54
Catechol	0.85	3	1.065	0.027	1.081	1.034	1.07
Resorcinol	1.10	8	1.001	0.055	1.062	0.833	1.00
Hydroquinone	1.16	9	0.999	0.127	1.154	0.705	1.00

(Continued on p. 130)

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
Methyl paraban	0.69	1	1.366				1.37
1-Naphthol	0.61	6	1.046	0.014	1.066	1.024	1.05
2-Naphthol	0.61	6	1.079	0.014	1.098	1.060	1.08
Benzyl alcohol	0.39	18	0.867	0.019	0.903	0.832	0.87
2-Methylbenzyl alcohol	0.39	2	0.897	0.016	0.908	0.885	0.90
3-Methylbenzyl alcohol	0.39	2	0.904	0.006	0.908	0.900	0.90
4-Methylbenzyl alcohol	0.39	2	0.885	0.006	0.889	0.880	0.89
2,4-Dimethylbenzyl alcohol	0.39	2	0.878	0.002	0.879	0.876	0.88
2,5-Dimethylbenzyl alcohol	0.39	2	0.878	0.008	0.883	0.872	0.88
3,4-Dimethylbenzyl alcohol	0.39	2	0.896	0.004	0.899	0.893	0.90
1-Phenylethanol	0.33	1	0.831				0.83
2-Phenylethanol	0.33	2	0.908	0.011	0.915	0.900	0.91
Thiophenol	0.09	16	0.802	0.028	0.899	0.777	0.80
Benzylthiol	0.00	1	0.788				0.79
Phenylmethylsulphide	0.00	1	0.918				0.92
Furan	0.00	1	0.525				0.53
Benzofuran	0.00	1	0.830				0.83
Dibenzofuran	0.00	3	1.018	0.033	1.043	0.980	1.02
Benzodioxane	0.00	3	1.073	0.049	1.128	1.035	1.07
Benzo[*kl*]xanthene	0.00	1	1.261				1.26
Trioxan	0.00	1	1.031				1.03
Pyridine	0.00	16	0.836	0.017	0.862	0.800	0.84
2-Methylpyridine	0.00	15	0.754	0.014	0.772	0.715	0.75
3-Methylpyridine	0.00	15	0.814	0.006	0.827	0.804	0.81
4-Methylpyridine	0.00	15	0.824	0.006	0.837	0.816	0.82
2-Ethylpyridine	0.00	13	0.708	0.009	0.723	0.694	0.71
3-Ethylpyridine	0.00	12	0.792	0.012	0.818	0.780	0.79
4-Ethylpyridine	0.00	14	0.804	0.010	0.826	0.789	0.80
2,3-Dimethylpyridine	0.00	9	0.769	0.007	0.778	0.757	0.77
2,4-Dimethylpyridine	0.00	10	0.759	0.008	0.776	0.748	0.76
2,5-Dimethylpyridine	0.00	8	0.743	0.005	0.753	0.737	0.74
2,6-Dimethylpyridine	0.00	10	0.696	0.034	0.767	0.636	0.70
3,4-Dimethylpyridine	0.00	8	0.854	0.015	0.877	0.830	0.85
3,5-Dimethylpyridine	0.00	6	0.794	0.007	0.804	0.786	0.79
2-*n*-Propylpyridine	0.00	7	0.699	0.008	0.714	0.692	0.70
3-*n*-Propylpyridine	0.00	3	0.785	0.018	0.803	0.767	0.78
4-*n*-Propylpyridine	0.00	7	0.767	0.005	0.774	0.760	0.77
4-Isopropylpyridine	0.00	3	0.757	0.008	0.766	0.752	0.76
2-Methyl-4-ethylpyridine	0.00	7	0.751	0.016	0.775	0.728	0.75
2-Methyl-5-ethylpyridine	0.00	6	0.705	0.035	0.754	0.663	0.71
2-Methyl-6-ethylpyridine	0.00	8	0.644	0.018	0.675	0.617	0.64
3-Methyl-2-ethylpyridine	0.00	2	0.717	0.013	0.726	0.708	0.72
3-Methyl-4-ethylpyridine	0.00	5	0.851	0.020	0.876	0.825	0.85
3-Methyl-5-ethylpyridine	0.00	3	0.807	0.013	0.820	0.794	0.81
3-Methyl-6-ethylpyridine	0.00	4	0.710	0.015	0.724	0.690	0.71
4-Methyl-2-ethylpyridine	0.00	5	0.725	0.009	0.738	0.713	0.73
4-Methyl-3-ethylpyridine	0.00	2	0.785	0.048	0.819	0.751	0.79
2,3,4-Trimethylpyridine	0.00	8	0.801	0.065	0.849	0.641	0.80
2,3,5-Trimethylpyridine	0.00	8	0.785	0.016	0.821	0.767	0.79
2,3,6-Trimethylpyridine	0.00	10	0.717	0.011	0.730	0.699	0.72
2,4,5-Trimethylpyridine	0.00	8	0.800	0.018	0.826	0.780	0.80
2,4,6-Trimethylpyridine	0.00	9	0.690	0.014	0.703	0.669	0.69
3,4,5-Trimethylpyridine	0.00	2	0.924	0.018	0.937	0.911	0.92

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
2-*n*-Butylpyridine	0.00	1	0.693				0.69
4-*tert.*-Butylpyridine	0.00	2	0.763	0.003	0.765	0.761	0.76
2,5-Diethylpyridine	0.00	2	0.699	0.008	0.704	0.693	0.70
2,6-Diethylpyridine	0.00	3	0.617	0.038	0.651	0.576	0.62
3,4-Diethylpyridine	0.00	2	0.814	0.004	0.816	0.811	0.81
3,5-Diethylpyridine	0.00	3	0.806	0.009	0.815	0.797	0.81
2-Methyl-4-propylpyridine	0.00	2	0.733	0.014	0.743	0.723	0.73
2-Methyl-5-propylpyridine	0.00	2	0.722	0.015	0.732	0.711	0.72
2-Methyl-6-propylpyridine	0.00	2	0.612	0.008	0.618	0.606	0.61
4-Methyl-2-propylpyridine	0.00	2	0.706	0.014	0.716	0.696	0.71
4-Methyl-3-propylpyridine	0.00	2	0.800	0.037	0.826	0.774	0.80
5-Methyl-2-propylpyridine	0.00	2	0.694	0.006	0.698	0.689	0.69
4-Methyl-3-isopropylpyridine	0.00	2	0.812	0.001	0.812	0.811	0.81
2,3-Dimethyl-4-ethylpyridine	0.00	3	0.757	0.158	0.875	0.578	0.76
2,3-Dimethyl-6-ethylpyridine	0.00	2	0.677	0.013	0.686	0.668	0.68
2,4-Dimethyl-5-ethylpyridine	0.00	4	0.805	0.030	0.831	0.778	0.80
2,4-Dimethyl-6-ethylpyridine	0.00	4	0.658	0.009	0.669	0.649	0.66
2,5-Dimethyl-4-ethylpyridine	0.00	4	0.789	0.025	0.816	0.763	0.79
2,5-Dimethyl-6-ethylpyridine	0.00	4	0.668	0.026	0.689	0.630	0.67
2,6-Dimethyl-3-ethylpyridine	0.00	4	0.695	0.008	0.706	0.686	0.69
2,6-Dimethyl-4-ethylpyridine	0.00	4	0.702	0.020	0.718	0.674	0.70
3,4-Dimethyl-6-ethylpyridine	0.00	2	0.773	0.014	0.783	0.763	0.77
3,5-Dimethyl-6-ethylpyridine	0.00	3	0.724	0.022	0.741	0.700	0.72
2,3,4,5-Tetramethylpyridine	0.00	1	0.845	0.000	0.845	0.845	0.84
2,3,4,6-Tetramethylpyridine	0.00	5	0.755	0.012	0.767	0.737	0.76
2,3,5,6-Tetramethylpyridine	0.00	4	0.768	0.058	0.852	0.721	0.77
2-*n*-Pentylpyridine	0.00	2	0.635	0.081	0.692	0.578	0.64
4-*n*-Pentylpyridine	0.00	2	0.568	0.010	0.575	0.561	0.57
2-Methyl-6-butylpyridine	0.00	2	0.545	0.024	0.562	0.528	0.55
2-Ethyl-6-propylpyridine	0.00	2	0.547	0.004	0.550	0.544	0.55
2-Methyl-4,5-diethylpyridine	0.00	2	0.849	0.021	0.864	0.834	0.83
2-Methyl-4,6-diethylpyridine	0.00	4	0.646	0.013	0.663	0.635	0.65
2-Methyl-5,6-diethylpyridine	0.00	2	0.659	0.032	0.681	0.636	0.66
4-Methyl-2,6-diethylpyridine	0.00	2	0.593	0.002	0.594	0.591	0.59
2,6-Dimethyl-4-propylpyridine	0.00	2	0.656	0.004	0.658	0.653	0.66
2-Isopropyl-3,6-dimethylpyridine	0.00	2	0.579	0.010	0.586	0.572	0.58
2,3,6-Trimethyl-4-ethylpyridine	0.00	2	0.696	0.011	0.703	0.688	0.70
2,4,6-Trimethyl-3-ethylpyridine	0.00	4	0.742	0.053	0.804	0.689	0.74
2,4,6-Triethylpyridine	0.00	2	0.531	0.020	0.545	0.517	0.54
2,3-Dimethyl-4,6-diethylpyridine	0.00	2	0.769	0.029	0.789	0.748	0.77
2,5-Dimethyl-4,6-diethylpyridine	0.00	2	0.778	0.030	0.799	0.757	0.78
3,4-Dimethyl-2,6-diethylpyridine	0.00	2	0.605	0.032	0.627	0.582	0.61
2-(5-Nonyl)pyridine	0.00	2	0.486	0.034	0.510	0.462	0.49
4-(5-Nonyl)pyridine	0.00	2	0.487	0.024	0.504	0.470	0.49
2-Benzylpyridine	0.00	1	0.809				0.81
4-Benzylpyridine	0.00	1	0.797				0.80
Cyclopenteno[*b*]pyridine	0.00	2	0.905	0.007	0.910	0.900	0.90
2-Methylcyclopenteno[*b*]pyridine	0.00	2	0.774	0.012	0.782	0.765	0.77
4-Methylcyclopenteno[*b*]pyridine	0.00	1	0.844				0.84
7-Methylcyclopenteno[*b*]pyridine	0.00	2	0.802	0.001	0.803	0.801	0.80
Cyclopenteno[*c*]pyridine	0.00	2	0.942	0.013	0.951	0.933	0.94

(Continued on p. 132)

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
3-Methylthiopyridine	0.00	2	1.135	0.030	1.156	1.113	1.13
2-Fluoropyridine	0.00	1	0.890				0.89
3-Fluoropyridine	0.00	1	0.739				0.74
4-Fluoropyridine	0.00	1	0.773				0.77
2-Chloropyridine	0.00	1	1.026				1.03
3-Chloropyridine	0.00	1	0.834				0.83
4-Chloropyridine	0.00	1	0.848				0.85
2-Bromopyridine	0.00	1	1.056				1.06
3-Bromopyridine	0.00	1	0.895				0.90
4-Bromopyridine	0.00	1	0.931				0.93
2-Iodopyridine	0.00	1	1.105				1.10
3-Iodopyridine	0.00	1	0.978				0.98
4-Iodopyridine	0.00	1	0.968				0.97
3-Methoxypyridine	0.00	1	0.945				0.95
4-Methoxypyridine	0.00	1	0.932				0.93
2-Cyanopyridine	0.00	1	1.437				1.44
3-Cyanopyridine	0.00	1	1.264				1.26
4-Cyanopyridine	0.00	1	1.207				1.21
2-Nitropyridine	0.00	1	1.421				1.42
3-Nitropyridine	0.00	1	1.280				1.28
4-Nitropyridine	0.00	1	1.211				1.21
Piperidine	0.10	2	0.463	0.004	0.466	0.460	0.46
N-Methylpiperidine	0.00	3	0.386	0.081	0.480	0.334	0.39
N-Ethylpiperidine	0.00	2	0.315	0.004	0.318	0.312	0.32
Quinoline	0.00	9	0.965	0.032	1.027	0.916	0.97
1,2,3,4-Tetrahydroquinoline	0.00	1	0.943				0.94
2-Methylquinoline	0.00	3	0.877	0.035	0.917	0.854	0.88
4-Methylquinoline	0.00	4	0.978	0.020	0.999	0.951	0.98
6-Methylquinoline	0.00	5	0.948	0.017	0.974	0.931	0.95
7-Methylquinoline	0.00	1	0.949				0.95
8-Methylquinoline	0.00	5	0.867	0.033	0.911	0.829	0.87
2,3-Dimethylquinoline	0.00	1	1.009				1.01
2,4-Dimethylquinoline	0.00	4	0.957	0.020	0.983	0.939	0.96
2,6-Dimethylquinoline	0.00	4	0.898	0.012	0.912	0.882	0.90
2,4,6-Trimethylquinoline	0.00	1	0.995				1.00
2,4,6,8-Tetramethylquinoline	0.00	1	0.941				0.94
Isoquinoline	0.00	9	0.998	0.034	1.056	0.953	1.00
1,2,3,4-Tetrahydroisoquinoline	0.00	1	0.904				0.90
1-Methylisoquinoline	0.00	1	1.025				1.02
3-Methylisoquinoline	0.00	6	0.897	0.050	0.970	0.822	0.90
Benzo[*c*]quinoline	0.00	4	1.254	0.046	1.295	1.212	1.25
Benzo[*f*]quinoline	0.00	2	1.252	0.008	1.257	1.246	1.25
3-Methylbenzo[*f*]quinoline	0.00	1	0.979				0.98
Benzo[*h*]quinoline	0.00	2	1.215	0.019	1.228	1.201	1.22
Acridine	0.00	4	1.325	0.030	1.370	1.304	1.32
2-Methylacridine	0.00	1	1.055				1.06
3-Methylacridine	0.00	1	1.108				1.11
Benz[*a*]acridine	0.00	2	1.577	0.009	1.583	1.570	1.58
10-Methylbenz[*a*]acridine	0.00	1	1.700				1.70
Benz[*c*]acridine	0.00	3	1.516	0.030	1.537	1.481	1.52
10-Methylbenz[*c*]acridine	0.00	1	1.689				1.69
1,10-Dimethylbenz[*c*]acridine	0.00	1	1.568				1.57
2,10-Dimethylbenz[*c*]acridine	0.00	1	1.583				1.58

TABLE III *(continued)*

Solute	α_2^H	No.	Average	S.D.	Max	Min	Taken
Pyrrole	0.41	2	0.731	0.049	0.766	0.696	0.73
N-Methylpyrrole	0.00	1	0.792				0.79
N-Methylpyrrolidine	0.00	1	0.497				0.50
Indole	0.44	7	1.125	0.047	1.178	1.047	1.12
N-Methylindole	0.00	1	0.922				0.92
2-Methylindole	0.44	2	1.054	0.011	1.061	1.046	1.05
3-Methylindole	0.44	5	1.058	0.015	1.076	1.037	1.06
5-Methylindole	0.44	4	1.082	0.024	1.115	1.060	1.08
7-Methylindole	0.44	1	1.049				1.05
2,N-Dimethylindole	0.00	2	0.961	0.008	0.967	0.955	0.96
2,3-Dimethylindole	0.44	1	1.005				1.01
2,5-Dimethylindole	0.44	1	1.029				1.03
2,7-Dimethylindole	0.44	2	1.050	0.068	1.098	1.002	1.05
2,3,7-Trimethylindole	0.44	2	1.106	0.059	1.148	1.064	1.11
Carbazole	0.47	4	1.423	0.028	1.447	1.388	1.42
2-Methylcarbazole	0.47	2	1.384	0.006	1.388	1.379	1.38
Pyrazole	0.54	1	0.995				1.00
3-Methylpyrazole	0.54	1	0.876				0.88
4-Methylpyrazole	0.54	1	0.991				0.99
Thiophene	0.00	1	0.565				0.57
2-Methylthiophene	0.00	1	0.561				0.56
2,5-Dimethylthiophene	0.00	1	0.538				0.54
Tetrahydrothiophene	0.00	1	0.528				0.53
Benzo[*b*]thiophene	0.00	2	0.881	0.039	0.908	0.853	0.88
Dibenzothiophene	0.00	1	1.308				1.31
Benz[*b*]naphtho[2,1-*d*]thiophene	0.00	1	1.561				1.56

TABLE IV

COMPARISON OF π_2^H VALUES WITH THOSE FROM RESULTS OF POOLE AND CO-WORKERS [86,87]

Solute	Table III			Poole and co-workers
	π_2^H	S.D.	No.	π_2^H
Anisole	0.745	0.026	30	0.768
Benzonitrile	1.110	0.019	21	1.125
Aniline	0.960	0.023	29	0.972
N-Methylaniline	0.898	0.020	10	0.892
N,N-Dimethylaniline	0.842	0.016	11	0.829
Nitrobenzene	1.108	0.019	20	1.113
Phenol	0.892	0.020	46	0.909
2,4,6-Trimethylphenol	0.791	0.033	11	0.820

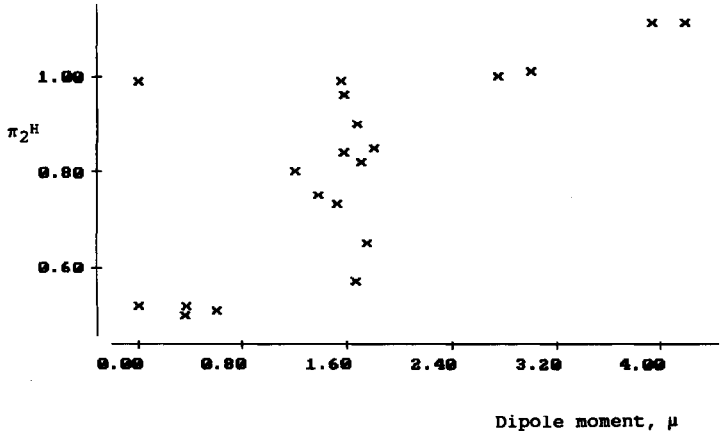

Fig. 1. Plot of π_2^H *vs.* dipole moment, μ, for solutes in Table II.

If μ is replaced by the calculated dipole moment, μ^c, *i.e.* calculated by vectorial summation taking μ for chlorobenzene as 1.72 D, then eqn. 15 results,

$$\pi_2^H = 0.541 + 0.0750nCl + 0.0252\mu^c$$
$$n = 13 \quad \rho = 0.982 \quad \text{S.D.} = 0.027 \qquad (15)$$

In both eqn. 14 and eqn. 15 the major contribution is made by the term in nCl, suggesting that polarisability is a much larger factor than dipole moment. A similar equation results from an analysis of the chloroanisoles, provided that all 2,6-dichloroanisoles are left out,

$$\pi_2^H = 0.717 + 0.0856nCl + 0.0375\mu^c$$
$$n = 14 \quad \rho = 0.965 \quad \text{S.D.} = 0.030 \qquad (16)$$

If the number of chlorine substituents is the major factor affecting π_2^H, as in eqns. 14–16, then simple summation of substituent constants might yield reasonable estimates of π_2^H, at least for disubstituted solutes. Results are in Table V, using the substituent constants in Table II, $\Delta\pi_2^H$, together with an adjustment for *meta*-substituted compounds by a factor of 0.94 and one for para-substituted compounds by a factor of 0.96. For halogen substituted compounds, except those of aniline and phenol, there is reasonable agreement between calculated and observed π_2^H values. Hence the calculated values for the substituents Br/OMe, I/OMe, Cl/CO_2Me, F/NO_2, Br/NMe_2 and probably also Cl/NHMe can be taken as reasonable estimates of π_2^H. There seems no reason why π_2^H values for the substituents Br/CO_2Me, I/CO_2Me, Br/NO_2, I/NO_2, Br/NHMe (*m* and *p* only) and I/NMe_2 cannot be similarly calculated.

For polyhalogenated compounds a rather more elaborate treatment is required, based on equations such as eqn. 15. Analysis of the various π_2^H values for halogen substituents leads to the $n(n\text{X})$ and $m(\mu^c)$ values in Table VI that correspond to equations like that of eqn. 15. The π_2^H value for any polyhalogenated compound is given by

$$\pi_2^H = 0.52 + n \cdot n'(\text{X}) + n'(\text{Y}) + m'\mu^c \qquad (17)$$

where n is the number of halogen substituents, n'(X) is the value listed in Table VI for the halogen concerned, n'(Y) is the value listed in Table VI for the other (single) substituent, μ^c is the calculated overall dipole moment, and m' is the average of the *m*-values in Table VI. For example, in 2,5-dichloro methylbenzoate[a] $n = 2$, $n'(\text{X}) = 0.0750$, $n'(\text{Y}) = 0.2940$, $\mu^c = 1.80$ D using the dipole moments in Table II, and $m' = (2 \times 0.0252 + 0.0200)/3 = 0.023$ units. In Table VII are results on these lines. There is good agreement with experiment, except for 3-chloroveratrole and 3,4–dichloroveratrole where there are substituents in the 1,2,3-positions (cf. the exceptions to eqn. 16). Agreement is possibly even better if a correction factor is again used for the case of meta substituted com-

[a] Listed as methyl 2,5-dichlorobenzoate in Tables II and III.

TABLE V

OBSERVED AND CALCULATED π_2^H VALUES FOR DIFUNCTIONAL BENZENES WITH ONE OR TWO HALOGEN SUBSTITUENTS

First line observed, second line calculated.

Substituents	*Ortho*[a]	*Meta*	*Para*	Substituents	*Ortho*[a]	*Meta*	*Para*
F/F	0.75			Cl/NO_2	1.25	1.13	1.17
	0.62	0.58[b]	0.60[c]		1.24	1.17[b]	1.19[c]
Cl/Cl	0.78	0.73	0.75	Cl/NHMe	0.96		1.01
	0.78	0.73[b]	0.75[c]		1.03	0.97[b]	0.99[c]
Br/Br	0.96	0.88	0.86	Br/NMe_2			0.97
	0.94	0.88[b]	0.90[c]		1.05	0.99[b]	1.01[c]
I/I	1.21	1.07	1.15	F/NH_2	0.88	1.08	1.09
	1.12	1.05[b]	1.08[c]		1.01		
F/OMe	0.79	0.72	0.74	Cl/NH_2	0.92	1.10	1.13
	0.80	0.75[b]	0.77[c]		1.09		
Cl/OMe	0.91	0.86	0.86	Br/NH_2	0.98	1.19	1.19
	0.88	0.83[b]	0.85[c]		1.17		
Br/OMe			0.90	I/NH_2	1.00	1.26	1.28
	0.96	0.90[b]	0.92[c]		1.26		
I/OMe			0.99	F/OH	0.69	0.98	0.95
	1.05	0.99[b]	1.01[c]		0.94		
F/CO_2Me	0.89	0.88	0.89	Cl/OH	0.86	1.06	1.08
	0.90	0.85[b]	0.86[c]		1.04		
Cl/CO_2Me	0.99		0.92	Br/OH	0.90	1.15	1.17
	0.98	0.92[b]	0.94[c]		1.10		
Cl/CN	1.24	1.14	1.18	I/OH	1.00	1.20	1.33
	1.24	1.16[b]	1.19[c]		1.19		
F/NO_2		1.11					
	1.16	1.09[b]	1.11[c]				

[a] All *ortho* values calculated by simple summation.
[b] Taken as 94% of the calculated *ortho* value.
[c] Taken as 96% of the calculated *ortho* value.

TABLE VI

VALUES OF n' AND m' IN EQN. 17

Substituent	n'	m'
F	0.0241	0.0132
Cl	0.0750	0.0252
Br	0.1670	0.0349
I	0.2710	0.0128
OMe	0.2028	0.0158
COMe	0.4300	0.0200
CO_2Me	0.2940	0.0200
CN	0.5064	0.0200
NO_2	0.5114	0.0200
CHO	0.4250	0.0200
NMe_2	0.2886	0.0200

pounds. For these calculations a factor of 0.96 for *meta*-substituted C_6H_5XY compounds seems appropriate. A rather large number of π_2^H values for halogeno-substituted derivatives of PhY where Y = (F), Cl, Br, I, OMe (in part), CHO, COMe, CO_2Me, CN, NO_2 and NMe_2 can be estimated using eqn. 17.

Halogeno derivatives of phenol and aniline behave quite differently to those of the above compounds, as shown quite clearly by results in Table V. Not only do the *ortho*-halogeno compounds have π_2^H lower than calculated by simple summation, but the *meta*- and *para*-derivatives have π_2^H values larger than calculated. For both series, π_2^H values are known for all the isomers

TABLE VII
CALCULATION OF π_2^H FOR HALO-AROMATICS VIA EQN. 17

Solute	π_2^H	
	Observed	Calculated
3-Chloroveratrole	0.96	1.06
4-Chloroveratrole	1.03	1.02
3,4-Dichloroveratrole	1.05	1.13
4,5-Dichloroveratrole	1.11	1.08
2-Chloro methylbenzoate	0.96	0.99
4-Chloro methylbenzoate	0.89	0.92
2,4-Dichloro methylbenzoate	0.98	1.01
2,5-Dichloro methylbenzoate	0.99	1.01
2-Fluoro methylbenzoate	0.89	0.89
3-Fluoro methylbenzoate	0.88	0.87
4-Fluoro methylbenzoate	0.89	0.84
2-Chlorobenzonitrile	1.24	1.22
3-Chlorobenzonitrile	1.14	1.19(1.14)[a]
4-Chlorobenzonitrile	1.16	1.11
2-Chloronitrobenzene	1.24	1.22
3-Chloronitrobenzene	1.14	1.18(1.13)[a]
4-Chloronitrobenzene	1.18	1.16
4-Bromoanisole	0.90	0.89
4-Iodoanisole	0.99	0.99
4-Bromo-N,N-dimethylamine	0.97	0.98

[a] Using a factor of 0.96 for *m*-substituents, see text.

of all the halogens in the monohalogenated derivatives, so no estimations here are needed. It would be helpful to be able to estimate π_2^H values for the polyhalogenated compounds, but there are not enough data to attempt this.

Such is the case also with disubstituted (and polysubstituted) compounds where neither substituent is halogen. Again, there are not enough data to come to any general conclusion as to how π_2^H varies with di- and poly-substitution. Further results are needed, and it is hoped that data will be obtained in the near future.

There is a reasonable amount of data, however, for substituted pyridines, especially the monosubstituted ones. In Table VIII are collected π_2^H values for 2-, 3- and 4-substituted pyridines, taken from Table III, together with the aromatic $\Delta\pi_2^H$ substituent constants from Tables II and III. If the aromatic $\Delta\pi_2^H$ constants are applied to the substituted pyridine, with π_2^H equal to 0.84 for pyridine itself, the calculated π_2^H values for the pyridine are as given also in Table VIII. The trends in these calculated values can be seen more clearly by setting out values of π_2^H (calculated – observed), again given in Table VIII. There is a clear separation between the alkyl substituents and the others. In the former case, π_2^H for the 2-alkylpyridines is always lower than for the corresponding 3- and 4-alkylpyridines, leading to π_2^H (calculated – observed) around 0.12 units for the higher alkyl groups. The π_2^H (calculated – observed) values seem quite regular, and allow the estimation of further values, given in parentheses in Table VIII.

For the other substituents shown in Table VIII, there are again general trends, but now π_2^H for the 2-substituent is usually larger than for the 3- or 4-substituents. If the remaining 2-substituents in Table VIII show the same trend, then π_2^H values for various 2-substituted pyridine can be found by simple addition using the aromatic substituent constants in Table II. Note that for the six nonalkyl 2-substituted pyridines in Table VIII, π_2^H(observed – calculated) averages as −0.01 unit, so when the estimated π_2^H (observed – calculated) values are taken as zero (*i.e.* simple addition obtains), the corresponding π_2^H values themselves can be calculated.

In the case of the (nonalkyl) 3- and 4-substituted pyridines in Table VIII, the value of π_2^H (calculated – observed) depends slightly on π_2^H itself. Estimated values of π_2^H (calculated – observed) are given, taking into account this dependency, and from these values, then π_2^H values for 3- and 4-substituted pyridine can be obtained as shown. There is not enough data available to estimate π_2^H values for polysubstituted pyridines, other than for polyalkylated ones, but at least there are now available π_2^H values or estimated π_2^H values for a quite wide range of 2-, 3- and 4-substituted pyridines.

Finally, we note that Li *et al.* [100] have constructed a scale of π_2^C values using a similar equation to eqn. 1 except that the old-fashioned δ_2 parameter [101] is retained instead of the R_2 parameter. Because the defining equation for π_2^C is not the same as the defining equation for π_2^H, these two parameters are not interchangeable, and cannot simply be transformed into each other. The π_2^H parameter must be used in combi-

TABLE VIII

CALCULATION OF π_2^H FOR MONOSUBSTITUTED PYRIDINES

Calculated π_2^H obtained using π_2^H of 0.84 for pyridine, and the aromatic substituent constants in Table II or from ref. 5. Estimated π_2^H (calculated – observed) and estimated π_2^H values are in parentheses.

Substituent	π_2^H (observed)			π_2^H (calculated)	π_2^H (calculated – observed)		
	2	3	4		2	3	4
Me	0.75	0.81	0.82	0.84	0.09	0.03	0.02
Et	0.70	0.79	0.80	0.83	0.13	0.04	0.03
Pr	0.70	0.79	0.77	0.82	0.12	0.03	0.05
Pr^{iso}	(0.68)	(0.78)	0.76	0.81	(0.13)	(0.03)	0.05
Bu	0.69	(0.80)	(0.78)	0.83	0.14	(0.03)	(0.05)
$Bu^{tert.}$	(0.67)	(0.78)	0.76	0.81	(0.14)	(0.03)	0.05
Pe	0.64		0.57	0.83	0.19		0.26
F	0.89	0.74	0.77	0.89	0.00	0.15	0.12
Cl	1.03	0.83	0.85	0.97	−0.06	0.14	0.12
Br	1.06	0.90	0.93	1.05	−0.01	0.15	0.12
I	1.11	0.98	0.97	1.14	0.03	0.16	0.17
MeO		0.94	0.93	1.07		0.13	0.14
CN	1.44	1.26	1.21	1.43	−0.01	0.17	0.22
NO_2	1.42	1.28	1.21	1.43	0.01	0.15	0.22
CO_2Me	(1.17)	(1.07)	(1.01)	1.17	(0.00)	(0.15)	(0.16)
CO_2H	(1.22)	(1.07)	(1.05)	1.22	(0.00)	(0.15)	(0.17)
HCO	(1.32)	(1.16)	(1.12)	1.32	(0.00)	(0.16)	(0.20)
CH_3CO	(1.33)	(1.17)	(1.13)	1.33	(0.00)	(0.16)	(0.20)
$CONH_2$	(1.82)	(1.65)	(1.60)	1.82	(0.00)	(0.17)	(0.22)
NH_2	–	(1.13)	(1.10)	1.28	–	(0.15)	(0.18)
NMe_2	–	(1.01)	(1.00)	1.16	–	(0.15)	(0.16)
CH_2OH	–	(1.04)	(1.02)	1.19	–	(0.15)	(0.17)

nation with R_2, as in the general solvation eqn. 1, whereas the π_2^C parameter must be used together with δ_2.

As far as the generality of eqn. 1 is concerned, this lack of transferability is not a problem since there are now available, from this work and previous work [1,5], around 1000 values of π_2^H. The π_2^H scale can now be regarded as reasonably well-established, and further values for, *e.g.* multifunctional aromatic compounds can in principle be obtained by the methods outlined in the present work.

REFERENCES

1 M.H. Abraham, G.S. Whiting, R.M. Doherty and W.J. Shuely, *J. Chromatogr.*, 587 (1991) 213.
2 M.H. Abraham, G.S. Whiting, R.M. Doherty and W.J. Shuely, *J. Chromatogr.*, 587 (1991) 229.
3 M.H. Abraham, I. Hamerton, J.B. Rose and J.W. Grate, *J. Chem. Soc., Perkin Trans. 2*, (1990) 1451.
4 M.H. Abraham, G.S. Whiting, J. Andonian-Haftvan and J.W. Steed, *J. Chromatogr.*, 588 (1991) 361.
5 M.H. Abraham and G.S. Whiting, *J. Chromatogr.*, 594 (1992) 229.
6 M.H. Abraham and D.V. Walsh, *J. Chromatogr.*, 627 (1992) 294.
7 M.H. Abraham, G.S. Whiting, R.M. Doherty, W.J. Shuely and P. Sakellariou, *Polymer*, 33 (1992) 2163.
8 M.H. Abraham and G.S. Whiting, *J. Am. Oil. Chem. Assoc.*, 69 (1992) 1236.
9 M.H. Abraham, P.L. Grellier and R.A. McGill, *J. Chem. Soc., Perkin Trans. 2*, (1987) 797.
10 M.H. Abraham, G.S. Whiting, R.M. Doherty and W.J. Shuely, *J. Chem. Soc., Perkin Trans. 2*, (1990) 1451.
11 I.O.O. Korhonen and J. Knuutinen, *J. Chromatogr.*, 292 (1984) 345.
12 I.O.O. Korhonen, J. Knuutinen and R. Jaaskelainen, *J. Chromatogr.*, 287 (1984) 293.
13 I.O.O. Korhonen, *J. Chromatogr.*, 294 (1984) 99.
14 I.O.O. Korhonen, *J. Chromatogr.*, 315 (1984) 185.

15 I.O.O. Korhonen and M.A. Lind, *J. Chromatogr.*, 322 (1985) 71.
16 I.O.O. Korhonen and M.A. Lind, *J. Chromatogr.*, 322 (1985) 83.
17 I.O.O. Korhonen and M.A. Lind, *J. Chromatogr.*, 328 (1985) 325.
18 I.O.O. Korhonen, *J. Chromatogr.*, 356 (1986) 285.
19 I.O.O. Korhonen, *J. Chromatogr.*, 363 (1986) 277.
20 G.H.E. Nieuwdorp, C.L. de Ligny and N.G. van der Veen, *J. Chromatogr.*, 154 (1978) 133.
21 A.T. James, *Anal. Chem.*, 28 (1956) 1564.
22 J. Janak and R. Komers, in D.H. Desty (Editor), *Gas Chromatography 1958*, Butterworths, London, 1958, p. 343.
23 A. Wehrli and E. Kováts, *Helv. Chim. Acta*, 42 (1959) 2709.
24 D.H. Desty and C.L.A. Harbourn, *Anal. Chem.*, 31 (1959) 1965.
25 J. Janák and M. Hrivnac, *J. Chromatogr.*, 3 (1960) 297.
26 S.H. Langer, C. Zahn and G. Pantazoplos, *J. Chromatogr.*, 3 (1960) 154.
27 S.H. Langer and J.H. Purnell, *J. Phys. Chem.*, 67 (1963) 263.
28 J. Ratusky and L. Bastar, *Chem. Ind.*, (1964) 579.
29 V. Cantuti, G.P. Cartoni, A. Liberti and A.G. Torri, *J. Chromatogr.*, 17 (1965) 60.
30 A.C. Pronay, *J. Chromatogr.*, 18 (1965) 586.
31 E. Pillion, *J. Gas Chromatogr.*, 3 (1965) 239.
32 G. Alberini, V. Cantuti and G.P. Cartoni, in A.B. Littlewood (Editor), *Gas Chromatography 1966*, Butterworths, London, 1966, p. 258.
33 N. Carugno and S. Rossi, *J. Gas Chromatogr.*, 5 (1967) 103.
34 A.R. Cooper, C.W.P. Crowne and P.G. Farrell, *J. Chromatogr.*, 29 (1967) 1.
35 S.H. Langer, B.M. Johnson and J.R. Conder, *J. Phys. Chem.*, 72 (1968) 4020.
36 G.S. Giam, S.D. Abbott and W.B. Davis, *J. Chromatogr.*, 42 (1969) 457.
37 R.E. Poulson, *J. Chromatogr. Sci.*, 7 (1969) 152.
38 L.S. Bark and K.F. Clarke, *J. Chromatogr.*, 48 (1970) 418.
39 J. Hrivnak and J. Macak, *Anal. Chem.*, 43 (1971) 1039.
40 P.T. Mitchell and F. Vernon, *J. Chromatogr.*, 65 (1972) 487.
41 L.E. Cook and F.M Raushel, *J. Chromatogr.*, 65 (1972) 556.
42 V. Kusý, *Chemical Utilisation of Coal, Tar and Petroleum*, 11 (1971) 219.
43 J. Macak, P. Buryan and J. Hrivnak, *J. Chromatogr.*, 89 (1974) 309.
44 K. Tesarik and S. Ghyczy, *J. Chromatogr.*, 91 (1974) 723.
45 L.S. Bark and K.C. Wheatstone, *J. Chromatogr.*, 92 (1974) 281.
46 J. Kriz, M. Popl and J. Mostecky, *J. Chromatogr.*, 97 (1974) 3.
47 A.F. Shlyakhov, B.I. Anvaer, O.V. Zolotareva, N.N. Romina, N.V. Novikova and R.I. Koreshkova, *Zh. Anal. Khim.*, 30 (1975) 788.
48 S.D. West and R.C. Hall, *J. Chromatogr. Sci.*, 13 (1975) 5.
49 F. Vernon and G.T. Edwards, *J. Chromatogr.*, 110 (1975) 73.
50 G. Weissmann, *J. Chromatogr.*, 129 (1976) 431.
51 A.N. Korol, *J. Chromatogr.*, 129 (1976) 125.
52 I.L. Zhuravleva, Yu.P. Kapustin and R.V. Golovnya, *Zh. Anal. Khim.*, 31 (1976) 1378.
53 V.D. Shatts, A.A. Avots and V.A. Belikov, *Zh. Anal. Khim.*, 32 (1977) 797.
54 P. Buryan and J. Macak, *J. Chromatogr.*, 139 (1977) 69.
55 P. Buryan, J. Macak and J. Hrivnak, *J. Chromatogr.*, 139 (1977) 425
56 L.S. Lysyuk and A.N. Korol, *Chromatographia*, 10 (1977) 712.
57 L.G. Sednevets and A.G. Pankov, *Zh. Anal. Khim.*, 32 (1977) 1039.
58 A. Radecki and J. Grzybowski, *J. Chromatogr.*, 152 (1978) 211.
59 V.S. Kozlova and A.N. Korol, *Zh. Anal. Khim.*, 34 (1979) 2412.
60 V.M. Nabivarach and V.P. Dmitrikov, *Zh. Anal. Khim.*, 34 (1979) 2412.
61 M.L. Lee, D.L. Vassilaros, C.M. White and M. Novotny, *Anal. Chem.*, 51 (1979) 768.
62 A.N. Korol and N.V. Novorusskaya, *J. Chromatogr.*, 169 (1979) 73.
63 A. Radecki, J. Grzybowski, H. Lamparczyk and A. Nasal, *J. High Resolut. Chromatogr. Chromatogr. Commun.*, 2 (1979) 581.
64 W. Engewald, L. Wennrich and E. Ritter, *J. Chromatogr.*, 174 (1979) 315.
65 J. Grzybowski, H. Lamparczyk, A. Nasal and A. Radecki, *J. Chromatogr.*, 196 (1980) 217.
66 F. Sellier, G. Tersac and G. Guiochon, *J. Chromatogr.*, 219 (1981) 213.
67 V.A. Gerasimenko, A.V. Kirilenko and V.M. Nabivach, *J. Chromatogr.*, 208 (1981) 9.
68 C.M. White and N.C. Li, *Anal. Chem.*, 54 (1982) 1564.
69 F. Patte, M. Etcheto and P. Laffort, *Anal. Chem.*, 54 (1982) 2239.
70 D.L. Vassilaros, R.C. Kong, D.W. Later and M.L. Lee, *J. Chromatogr.*, 252 (1982) 1.
71 M. Novrocikova, J. Novrocik and J. Vymetal, *Collect. Czech. Chem. Commun.*, 48 (1983) 3270.
72 J.K Haken and I.O.O. Korhonen, *J. Chromatogr.*, 265 (1983) 323.
73 O. Buchman, G.-Y. Cao and C.T. Peng, *J. Chromatogr.*, 312 (1984) 75.
74 R. Fellous, L. Lizzani-Cuvelier and R. Luft, *Anal. Chim. Acta*, 174 (1985) 53.
75 K. Osmialowski, J. Halkiewicz and R. Kaliszan, *J. Chromatogr.*, 361 (1986) 63.
76 J. Oszczapowicz, K. Ciszkowski and J. Osek, *J. Chromatogr.*, 362 (1986) 383.
77 J. Bermeja, C.G. Blanco and M.D. Guillen, *J. Chromatogr.*, 351 (1986) 425.
78 J. Oszczapowicz, J. Osek, W. Krawczyk and B. Kielak, *J. Chromatogr.*, 357 (1986) 93.

79 U. Knecht and H.-J. Nitsch, *Fresenius' Z. Anal. Chem.*, 324 (1986) 142.
80 J.K. Haken and F. Vernon, *J. Chromatogr.*, 361 (1986) 57.
81 C.T. Peng, S.F. Ding, R.L. Hua and Z.C. Yang, *J. Chromatogr.*, 436 (1988) 137.
82 W. Engewald, U. Billing, I. Topalova and N. Petsev, *J. Chromatogr.*, 446 (1988) 71.
83 H.-B. Lee, *J. Assoc. Off. Anal. Chem.*, 71 (1988) 803.
84 C.G. Blanco, J. Blanco, J. Bermejo and M.D. Guillen, *J. Chromatogr.*, 465 (1989) 378.
85 N.R. Ayyangar, A.S. Tambe and S.S. Biswas, *J. Chromatogr.*, 483 (1989) 33.
86 B.R. Kersten, S.K. Poole and C.F. Poole, *J. Chromatogr.*, 468 (1989) 235.
87 C.F. Poole, R.M. Pomaville and T.A. Dean, *Anal. Chim. Acta*, 225 (1989) 193.
88 J. Krupcik, D. Repka, E. Benicka, T. Hevesi, J. Nolte, B. Paschold and H. Mayer, *J. Chromatogr.*, 448 (1988) 203.
89 I.L. Zhuraveleva, M.B. Terenina, V.V. Shenderyuk and R.V. Golovnya, *Zh. Anal. Khim.*, 45 (1990) 722.
90 G. Defayes, D.E. Fritz, T. Gorner, G. Huber, C. de Reyff and E. Kováts, *J. Chromatogr.*, 500 (1990) 139.
91 C.G. Blanco, J. Blanco, P. Bernard and M.D Guillen, *J. Chromatogr.*, 539 (1991) 157.
92 L.H. Wright and J.F. Walling, *J. Chromatogr.*, 540 (1991) 311.
93 D.T. Williams, Q. Tran, P. Fellin and K.A. Brice, *J. Chromatogr.*, 549 (1991) 297.
94 C.T. Peng, Z.C. Yang and S.F. Ding, *J. Chromatogr.*, 586 (1991) 85.
95 J.-C. Dutoit, *J. Chromatogr.*, 555 (1991) 191.
96 M.S. Vigdergauz and R.V. Vigalok, *Neftekhimiya*, 11 (1971) 144.
97 T. Toth, *Magy. Kém. Foly.*, 75 (1969) 245.
98 O.E. Schupp and J.S. Lewis (Editors), *Gas Chromatographia Data Compilation, Supplement 1*, American Society for Testing and Materials, Philadelphia, PA.
99 C.F. Poole, T.O. Kollie and S.K. Poole, *Chromatographia*, 34 (1992) 281.
100 J. Li, Y. Zhang, A.J. Dallas and P.W. Carr, *J. Chromatogr.*, 550 (1991) 101.
101 M.J. Kamlet, R.M. Doherty, J.-L.M. Abboud, M.H. Abraham and R.W. Taft, CHEMTECH, 16 (1986) 566.