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A Simple Method for Determining the Enthalpy of Specific Solute–Solvent Interaction

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Abstract—An equation correlating a parameter that described the enthalpy of nonspecific solvation of nonelectrolytes with a quantity characterizing intermolecular solute–solvent interaction was found. A simple and versatile method based on this equation was suggested for calculating the enthalpy of nonspecific solvation and the enthalpy of specific solute–solvent interaction.

The enthalpy of solvation of a solute A_i in a solvent S, $\Delta H_{\mathrm{solv}}^{A_i/S}$, is deteremined by the sum of all types of intermolecular solute–solvent interactions and by changes in the solvent–solvent interactions due to solvation (effect of cavity formation in a solvent). The enthalpy of solvation can be represented as a sum of the enthalpy of specific solute–solvent interactions, $\Delta H_{\mathrm{int}}^{A_i/S}$(sp.), and the enthalpy of nonspecific solvation, $\Delta H_{\mathrm{solv}}^{A_i/S}$(nonsp.):

$$\Delta H_{\mathrm{solv}}^{A_i/S} = \Delta H_{\mathrm{solv}}^{A_i/S}(\mathrm{nonsp.}) + \Delta H_{\mathrm{int}}^{A_i/S}(\mathrm{sp.}). \quad (1)$$

The best known methods for determination of the enthalpy of solute–solvent interactions are the Arnett's neat base method [1] and the method of baseline of inert solvents [2]. In both methods, the enthalpy of nonspecific solvation in Eq. (1) is estimated using a certain model compound. None of these methods substantiate the choice of the model compound.

This problem was largely solved within the framework of another method for separating out the enthalpy of specific interaction, the method of "basis compounds" [3–5]. However, the drawback of this method, compared to the two above-mentioned methods, is the need in a large body of experimental data on the enthalpies of solvation, to class a given substance with one or another group of related compounds.

In [6], we suggested a new method for calculating the enthalpy of nonspecific solvation, $\Delta H_{\mathrm{solv}}^{S_i/S}$(nonsp), of nonelectrolytes in various solvents using Eq. (2):

$$\Delta H_{\mathrm{solv}}^{A_i/S}(\mathrm{nonsp.}) = (\delta h_{\mathrm{cav}}^{S} - \delta h_{\mathrm{cav}}^{CH}) V_{\mathrm{ch}}^{A_i/CH} + q[(\Delta H_{\mathrm{solv}}^{A_i/TCM} - \Delta H_{\mathrm{solv}}^{A_i/CH}) - (\delta_{\mathrm{cav}}^{TCM} - \delta_{\mathrm{cav}}^{CH}) V_{\mathrm{ch}}^{A_i}, \quad (2)$$

where $\delta h_{\mathrm{cav}}^{S}$, $\delta h_{\mathrm{cav}}^{CH}$, and $\delta h_{\mathrm{cav}}^{TCM}$ are the specific relative enthalpies of cavity formation in a given solvent (S), cyclohexane (CH), and tetrachloromethane (TCM), respectively; $\Delta H_{\mathrm{solv}}^{A_i/CH}$ and $\Delta H_{\mathrm{solv}}^{A_i/TCM}$ are the enthalpies of solvation of a solute A_i in cyclohexane and tetrachloromethane, respectively; $V_{\mathrm{ch}}^{A_i}$ is the characteristic volume of the solute [7]. The coefficient q in [6] is considered as a variable parameter for each solvent; it shows by what factor the relative enthalpy of interaction of various solutes with a given solvent S exceeds the relative enthalpy of interaction with tetrachloromethane.

We performed calculations with Eq. (2) and determined the parameters q for 19 solvents. The experimental enthalpies of solvation of various substances in these solvents, and also in cyclohexane and tetrachloromethane were calculated from published data on the enthalpies of solution [2, 8–42] and enthalpies of vaporization [5, 12, 25, 27, 43–50]. Since Eq. (2) is intended for calculating the enthalpy of nonspecific solvation, we included only data for solutes that do not specifically interact with the solvent. We also excluded data on the enthalpies of solvation of triethylamine and pyridine, since there are indications [51] that solvation of these compounds in tetrachloromethane has a specific component. The solutes and parameters required for calculation with Eq. (2) are listed in Table 1. The characteristic volumes $V_{\mathrm{ch}}^{A_i}$ were taken from [52] or calculated according to [7]. The enthalpies of solvation in cyclohexane, $\Delta H_{\mathrm{solv}}^{A_i/CH}$, were calculated from published data on the enthalpies of solution [2, 11, 13, 15–18, 20, 25–27, 29, 33, 37, 39, 53, 54] and enthalpies of vaporization, $\Delta H_{\mathrm{vap}}^{A_i}$ [12, 16, 25, 27, 43, 44, 48–50, 55]; the enthalpies of solvation in tetrachloromethane, $\Delta H_{\mathrm{solv}}^{A_i/TCM}$, were calculated using data from [2, 12, 13, 16, 17, 20, 21, 23, 30, 31, 34, 36, 37, 39].

The parameters q calculated from Eq. (2) for various solvents are listed in Table 2. We included only

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Table 1. Characteristic volumes ($V_{\mathrm{ch}}^{\mathrm{A}_i}$), 100 cm^3 mol^{-1} units, enthalpies of vaporization ($\Delta H_{\mathrm{vap}}^{\mathrm{A}_i}$), and enthalpies of solvation in cyclohexane ($\Delta H_{\mathrm{solv}}^{\mathrm{A}_i/\mathrm{CH}}$) and tetrachloromethane ($\Delta H_{\mathrm{solv}}^{\mathrm{A}_i/\mathrm{TCM}}$), kJ mol^{-1}, for various solutes A$_i$

A_i	$V_{\mathrm{ch}}^{\mathrm{A}_i}$	$\Delta H_{\mathrm{vap}}^{\mathrm{A}_i}$	$-\Delta H_{\mathrm{solv}}^{\mathrm{A}_i/\mathrm{CH}}$	$-\Delta H_{\mathrm{solv}}^{\mathrm{A}_i/\mathrm{TCM}}$	A_i	$V_{\mathrm{ch}}^{\mathrm{A}_i}$	$\Delta H_{\mathrm{vap}}^{\mathrm{A}_i}$	$-\Delta H_{\mathrm{solv}}^{\mathrm{A}_i/\mathrm{CH}}$	$-\Delta H_{\mathrm{solv}}^{\mathrm{A}_i/\mathrm{TCM}}$
n-Pentane	0.8131	26.74	25.65	25.28	1,2-Dichlorobenzene	0.9612	47.70	42.48	46.15
n-Hexane	0.9540	31.55	30.42	29.92	1,4-Dichlorobenzene	0.9612	64.90	42.70	46.70
n-Heptane	1.0949	36.57	34.94	34.48	Diethyl ether	0.7309	27.15	25.11	28.91
n-Octane	1.2358	41.51	39.66	39.13	Dipropyl ether	1.0127	35.69	35.06	36.69
n-Nonane	1.3767	46.44	44.48	43.80	*iso*-Butyl ether	1.2945	44.69	43.14	45.65
n-Decane	1.5176	51.38	49.08	48.37	*tert*-Butyl methyl ether	0.8718	30.42	23.97	28.79
n-Dodecane	1.7990	61.30	58.41	57.66	THF	0.6223	32.01	28.62	34.52
n-Hexadecane	2.3630	81.38	77.32	76.69	1,4-Dioxane	0.6810	37.49	29.09	38.16
Cyclohexane	0.8454	33.05	33.05	32.34	Anisole	0.9160	46.82	39.62	45.27
2-Methylbutane	0.8131	25.23	24.60	23.93	Ethyl acetate	0.7466	35.14	27.86	34.97
2,2-Dimethyl butane	0.9540	27.70	27.15	25.90	Acetone	0.5470	31.30	21.55	28.60
1-Octene	1.1928	40.58	38.95	39.58	Butanone	0.6879	34.69	26.48	32.93
Benzene	0.7164	33.85	30.04	33.31	Pentan-2-one	0.8288	38.41	31.30	37.07
Toluene	0.8573	37.99	34.77	38.12	Hexan-2-one	0.9676	42.89	36.15	41.84
Ethylbenzene	0.9982	42.26	39.29	41.72	Heptan-2-one	1.1106	47.45	40.67	46.40
tert-Butylbenzene	1.2800	48.11	45.93	48.44	Heptan-4-one	1.1106	46.44	39.37	45.39
Mesitylene	1.1391	47.49	43.35	46.74	Octan-2-one	1.2515	51.80	45.00	50.65
Naphthalene	1.0854	72.89	49.89	54.14	Nonan-2-one	1.3924	56.61	50.01	55.19
Diphenyl	1.3242	81.60	57.80	63.06	Nonan-5-one	1.3924	54.89	48.89	54.43
Anthracene	1.4540	101.70	72.00	77.18	Cyclopentanone	0.7202	42.72	33.64	41.38
1-Chlorobutane	0.7946	33.51	30.54	33.18	Cyclohexanone	0.8611	45.06	37.66	44.68
trans-1,2-Dichloroethylene	0.5922	29.29	27.24	28.79	Benzaldehyde	0.8730	49.37	39.08	46.02
cis-1,2-Dichloroethylene	0.5922	30.96	26.91	29.33	Acetophenone	1.0139	53.39	42.66	50.08
Tetrachloromethane	0.7391	32.43	31.80	32.43	*N*,*N*-Dimethylaniline	1.0980	52.83	46.39	51.99
Fluorobenzene	0.7341	35.52	30.92	34.43	Nitrobenzene	0.8906	55.02	43.10	50.21
Chlorobenzene	0.8388	40.96	37.20	40.33	Acetonitrile	0.4042	32.93	17.43	25.36
Bromobenzene	0.8914	43.81	39.33	42.97	DMF	0.6468	47.70	34.10	44.52
Iodobenzene	0.9746	49.60	44.12	48.01	DMSO	0.6130	52.89	25.61	35.19

the solvents for which the number of experimental points N used in the calculation was no less than ten. We also give in Table 2 the correlation coefficients R and the standard deviations S_0 of the enthalpies of solvation calculated by Eq. (2) from the experimental values.

As already noted, q is a variable parameter found by linear regression from the experimental data on the enthalpies of solvation in each solvent. However, if q correlates with some other solvent parameters, it will become possible to estimate the enthalpy of nonspecific solvation of any solute in any solvent. We considered the correlations of q for various solvents with the Kirkwood function $(\varepsilon - 1)/(2\varepsilon + 1)$, Kamlet–Taft polarity–polarizability parameter π^*, Dimroth–Reichardt solvatochromic parameter $E_T(30)$, and Hildebrand parameter δ_{H}. The values of these four parameters for the solvents under consideration were taken from [56], and the correlations with q are shown in Fig. 1.

As seen from this figure, q shows certain correlation with the above parameters, but the quality of this correlation is insufficient to predict q for other solvents. Below are the respective correlation coefficients

Table 2. Correlation parameters[a] of Eq. (2) and specific relative enthalpies of cavity formation (δH^{S}_{cav}, 100 kJ cm^{-3} units) for various solvents

Solvent	N	R	S_0	q	δh^{S}_{cav}
Benzene	52	0.989	1.23	1.52 ± 0.03	5.02
Toluene	46	0.988	0.94	1.30 ± 0.03	2.65
n-Xylene	14	0.972	1.10	1.07 ± 0.07	1.31
Mesitylene	30	0.959	1.16	0.91 ± 0.05	1.10
1,2-Dichloroethane	42	0.990	1.57	2.28 ± 0.05	8.56
Chlorobenzene	15	0.992	0.80	1.22 ± 0.04	2.56
Trifluoromethylbenzene	28	0.990	0.94	1.52 ± 0.04	3.50
Dibutyl ether	27	0.945	0.88	0.56 ± 0.04	0.53
1,4-Dioxane	23	0.969	2.64	2.01 ± 0.11	7.58
Ehylacetate	44	0.977	1.93	1.70 ± 0.06	5.98
Acetone	25	0.985	1.92	1.94 ± 0.07	7.56
Triethylamine	28	0.910	1.05	0.51 ± 0.05	0.43
Nitrobenzene	12	0.990	1.44	1.60 ± 0.07	5.04
Acetonitrile	23	0.996	1.04	2.21 ± 0.04	10.22
Benzonitrile	16	0.998	0.64	1.84 ± 0.03	5.30
DMF	46	0.974	2.54	2.18 ± 0.08	8.78
Pyridine	20	0.993	1.37	1.92 ± 0.05	6.22
DMSO	42	0.971	3.23	2.47 ± 0.09	13.87

[a] (N) Number of points in sample, (R) correlation coefficient, and (S_0) standard deviation, kJ mol^{-1}.

and standard deviations of q: 0.681, 0.43; 0.797, 0.36; 0.848, 0.31; and 0.708, 0.41.

The correlation with one more solvent parameter, square root of the specific relative enthalpy of cavity formation, $(\delta h^{S}_{cav})^{1/2}$, is shown in Fig. 2. The sense of this correlation is as follows. The quantity q characterizes the capability of a solvent for additional dispersion interaction (relative to tetrachloromethane), and the specific relative enthalpy of cavity formation is the measure of solvent–solvent interactions. The specific relative enthalpies of cavity formation were calculated according to [57]; as the volume of solute (hexane), we took the McGowan characteristic volume (V_{ch}). The results are given in Table 1.

The parameters $(\delta h^{S}_{cav})^{1/2}$ and δ_H are similar in the physical sense, since in the regular solution theory the quantity δ^2_H is the measure of the energy of the cavity formation in a solvent. The difference is that the Hildebrand parameter reflects the averaged energy of all solvent–solvent interactions (as it is calculated from the enthalpy of vaporization), whereas the quantity $(\delta h^{S}_{cav})^{1/2}$ reflects only a part of the energy of intermolecular interactions. Namely, it is determined only by interactions whose break is required to accommodate an alkane molecule in the solvent matrix. For example, in associated solvents, in our opinion, the parameter $(\delta h^{S}_{cav})^{1/2}$ reflects mainly the energy of nonspecific solvent–solvent interactions.

Figure 2 shows that the correlation of q with this parameter is considerably better than with the parameters given in Fig. 1. The correlation coefficient is 0.984, and the standard deviation of calculated q from the experimental value is 0.11. Thus, the parameters q can be calculated by Eq. (3):

$$q = (0.20 \pm 0.07) + (0.65 \pm 0.03)(\delta h^{S}_{cav})^{1/2}. \qquad (3)$$

Having determined q from this correlation, we can calculate by Eqs. (2) and (3) the enthalpy of nonspecific solvation of any solute in any solvent. If a solute specifically interacts with a solvent, the difference between the experimental and calculated enthalpies of solvation will be a measure of specific interaction with the solvent. The combination of Eqs. (2) and (3) for calculating the enthalpy of specific interaction includes the difference between the enthalpies of solvation in the given solvent and cyclohexane, which is equal to the difference between the enthalpies of solution. Thus, the enthalpy of specific solute–solvent interaction, $\Delta H^{A_i/S}_{int}$(sp.), can be calculated by Eq. (4):

$$\begin{aligned}\Delta H^{A_i/S}_{int}(\text{sp.}) &= \Delta H^{A_i/S}_{s} - (\delta h^{S}_{cav} - \delta h^{CH}_{cav})V^{A_i}_{ch} - \Delta H^{A_i/CH}_{s} \\ &- [0.20 + 0.65(\delta h^{S}_{cav})^{1/2}][\Delta H^{A_i/TCM}_{s} - \Delta H^{A_i/CH}_{s}) \\ &- (\delta h^{TCM}_{cav} - \delta h^{CH}_{cav})V^{A_i}_{ch}, \qquad (4)\end{aligned}$$

where $\Delta H^{A_i/S}_{s}$ is the enthalpy of solution of substance A_i in solvent S. The quantities δh^{TCM}_{cav} and δh^{CH}_{cav} are the specific relative enthalpies of cavity formation in tetrachloromethane and cyclohexane, equal to 1.71 and 1.23, respectively. The quantity $V^{A_i}_{ch}$ is calculated by the simple additive scheme [7], and δh^{S}_{cav}, as the ratio of the enthalpy of solution of hexane in the given solvent to the characteristic volume of hexane. Thus, to calculate the enthalpy of specific solvation by Eq. (4), it is necessary to know the enthalpy of solution of a substance in the given solvent, cyclohexane, and tetrachloromethane, and also the enthalpy of solution of hexane (or any other *n*-alkane) in the given solvent. The latter three quantities are in most cases available from the literature.

To validate Eq. (4), we calculated with it the enthalpies of specific interaction for a series of solute–solvent combinations. As solutes we chose phenol and 4-fluorophenols, because for these compounds numerous data are available on the enthalpies of solution and enthalpies of hydrogen bonding with solvents. The enthalpies of specific interaction that we calcu-

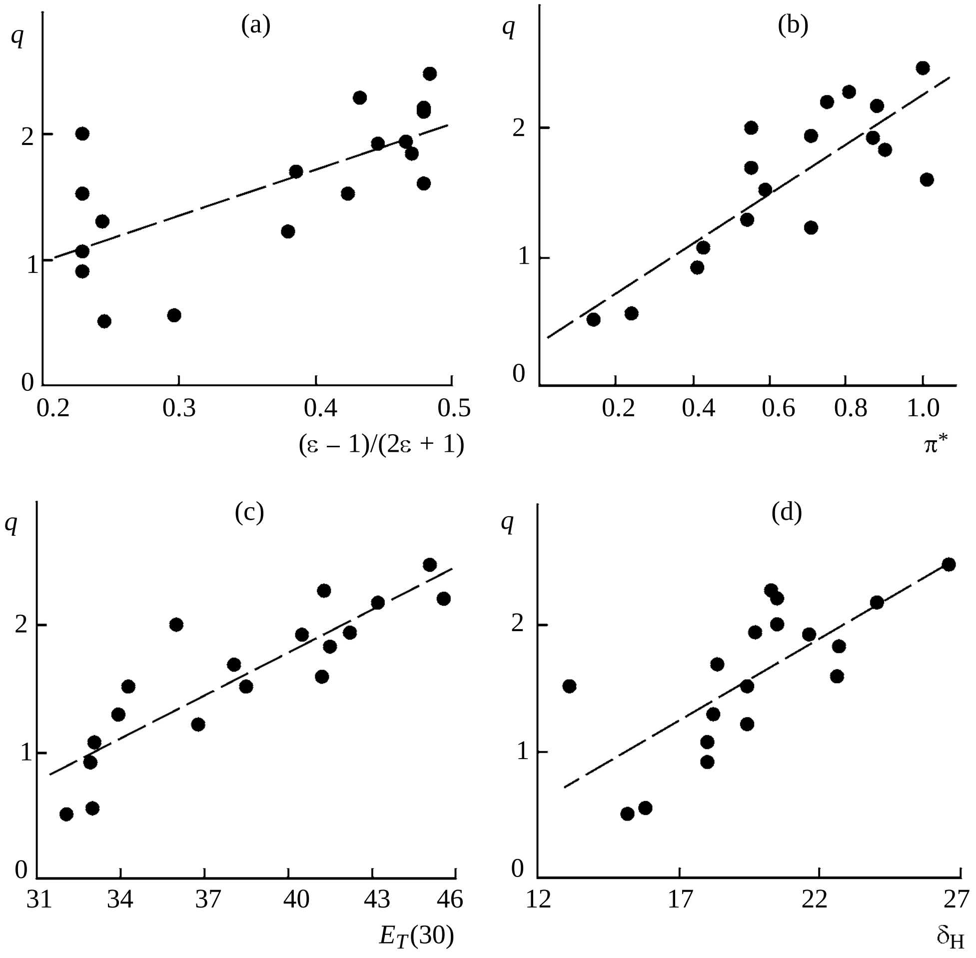

Fig. 1. Correlation of q for various solvents with the (a) Kirkwood function, (b) Kamlet–Taft polarity–polarizability parameter, (c) Dimroth–Reichardt parameter, and (d) Hildebrand parameter.

lated by Eq. (4) are listed in Table 3. The required data on the enthalpies of solution were taken from [4, 12, 23, 31, 40]. In the same table, we give for comparison the published data on the enthalpies of specific interaction with the solvent. It should be noted that available data on the enthalpies of hydrogen bonding of phenols with various proton acceptors are numerous but often contradictory. In Table 3 we give only a part of the published data, preferring the data that were obtained by calorimetric or spectral methods in an inert solvent (tetrachloromethane) or in a neat base.

The data for phenol show that the values obtained by Eq. (4) differ from the published data by no more than 2 kJ mol^{-1}, with the mean deviation being 0.92 kJ mol^{-1}. This deviation can be considered as insigificant, since the values reported by different authors in many cases differ more significantly.

The enthalpies of specific interaction of 4-fluoro-

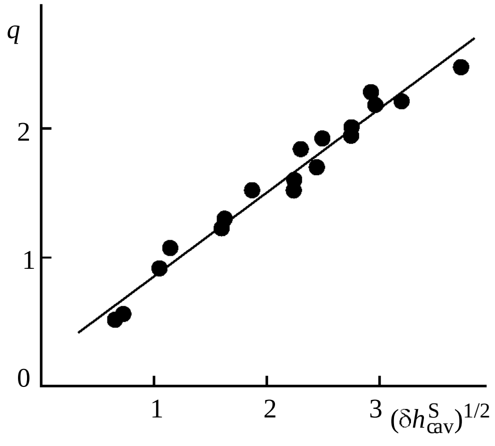

Fig. 2. Correlation of q for various solvents with the square root of the specific relative enthalpy of cavity formation $(\delta h^S_{cav})^{1/2}$, with the enthalpy measured in 100 kJ cm^{-3} units.

phenol with solvents differ from published data more significantly. The mean deviation in this case is 1.99 kJ mol^{-1}, with the values obtained by Eq. (4) being, as a rule, more negative. We believe that the certain systematic deviation in this case does not cast doubt on the validity of Eq. (4). It should be taken into account that virtually all published data on the enthalpies of hydrogen bonding of 4-fluorophenol [23, 31] were obtained by a single method, Arnett's neat base method. In accordance with this method, the enthalpy of a hydrogen bond is calculated as the difference between the enthalpies of transfer of a proton donor and a model compound from tetrachloromethane to the proton acceptor under consideration. As noted previously [4, 26, 32], the enthalpy of hydrogen bond obtained by this method may depend on the choice of the model compound. In [23, 31], the model compound was 4-fluoroanisole. However, our results [5, 20] show that anisole can also be a model compound in this case, since substitution of the hydrogen atom in the aromatic ring of the solute does not affect the type of nonspecific solvation and only slightly affects the molar refraction. We calculated the enthalpy of hydrogen bonding of 4-fluorophenol with some proton acceptors by the neat base method with anisole as model compound. These results are also given in the last column of Table 3, with supercript e. As seen, the enthalpies of hydrogen bonds obtained in this case are appreciably more negative.

Table 3. Enthalpies of specific interaction (kJ mol^{-1}), calculated by Eq. (4) and taken from the literature

Solvent	Enthalpy of specific interaction	
	Eq. (4)	data of other methods
	Phenol solute	
Benzene	–4.3	-6.9^{a} [58], -4.9^{b} [23]
Toluene	–6.1	-6.9^{a} [58], -5.5^{b} [23]
p-Xylene	–6.9	-9.0^{a} [58]
Mesitylene	–7.8	-8.0^{a} [58], -9.2^{a} [58]
1,4-Dioxane	–19.3	-20.9^{a} [58], -21.4^{b} [23]
Anisole	–11.9	-13.4^{a} [58], -12.9^{b} [23]
Ethyl acetate	–19.6	-20.1^{a} [58], -19.9^{b} [23]
Acetone	–21.0	-20.1^{b} [58], -19.7^{c} [58]
Pyridine	–29.2	-27.2^{b} [58], -30.5^{b} [23]
Acetonitrile	–13.4	-13.4^{c} [58], -17.8^{a} [58]
DMF	–27.6	-26.4^{b} [58], -28.7^{b} [23]
N,*N*-Dimethylacetamide	–30.1	-28.5^{b} [58], -30.8^{b} [23]
DMSO	–25.7	-27.2^{c} [58], -30.2^{b} [23]
	4-Fluorophenol solute	
Benzene	–5.7	-5.2^{b} [23], -6.6^{d}
Toluene	–7.9	-5.3^{b} [23]
Mesitylene	–10.2	-6.7^{b} [23], -9.3^{d}
1-Chlorobutane	–9.0	-8.1^{b} [23]
1-Bromobutane	–9.4	-7.6^{b} [23]
1,2-Dichlorobenzene	–3.0	-2.1^{b} [23]
Diethyl ether	–28.1	-23.4^{b} [23]
1,2-Dimethoxyethane	–28.2	-24.1^{b} [31]
1,4-Dioxane	–22.0	-20.1^{a} [59], -21.3^{b} [23]
Anisole	–13.4	-13.0^{b} [23], -14.4^{d}
Ethyl acetate	–22.1	-19.7^{e} [59], -19.8^{b} [23], -22.7^{d}
Propylene carbonate	–17.5	-19.0^{b} [23]
Acetone	–24.7	-23.4^{b} [31]
Cyclohexanone	–26.3	-24.3^{b} [23], -23.8^{b} [23]
Triethylamine	–42.2	-37.3^{b} [23]
Pyridine	–30.7	-29.7^{a} [23], -30.9^{b} [23]
DMF	–30.9	-27.6^{a} [23], -29.2^{b} [23], -32.6^{d}
N,*N*-Dimethylacetamide	–33.6	-28.5^{a} [60], -31.1^{b} [23]
DMSO	–28.7	-27.6^{a} [23], -30.2^{b} [23], -33.1^{d}

Note: The enthalpies of the hydrogen bond, given in the last column, were determined by the following methods: ^{a} IR spectroscopy; ^{b} calorimetry; ^{c} UV spectroscopy; ^{d} calculated in this work from the calorimetric data using the neat base method [23], with anisole taken as model compound; ^{e} NMR spectroscopy.

We believe that this example demonstrates one of advantages of our method. Equation (4) involves no model compound in the explicit form, but actually the model compounds are the solutes listed in Table 1, for which the enthalpy of nonspecific solvation is described by general equation (2). This decreases the probability of errors originating from improper choice of a model compound or from inaccurate determination of its enthalpy of solution.

A significant advantage of our method is the possibility of calculating the enthalpy of specific solute–solvent interaction from the minimal set of data on the enthalpies of solution. Furthermore, calculations by this equation do not require knowledge of the enthalpy of vaporization of the solute, necessary for calculating the enthalpies of solvation in the method of "basis compounds."

EXPERIMENTAL

The experimental enthalpies of solution were taken from [2, 8–42].

The enthalpies of solvation required for calculations with Eq. (2) were determined as the differences between the enthalpies of solution and enthalpies of vaporization [5, 12, 16, 25, 27, 43, 44, 48–50, 55]:

$$\Delta H_{\text{solv}}^{\text{A}_i/\text{S}} = \Delta H_{\text{s}}^{\text{A}_i/\text{S}} - \Delta H_{\text{vap}}^{\text{A}_i/\text{S}}. \quad (5)$$

If published data were contradictory, we preferred the results obtained calorimetrically or the results of later studies.

The enthalpies of formation of a hydrogen bond of a solute with a solvent were taken from [23, 31, 58–60]. If published data were contradictory, we preferred the results obtained calorimetrically or spectroscopically in an inert solvent (tetrachloromethane) or in a neat base.

To perform the statistical calculations by Eq. (2) and determine the parameters of linear correlation of various solvent properties with each other, we used the SPSS program (version 8).

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