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Thermochemistry of Dissolution, Solvation, and Hydrogen Bonding of Anilines in Proton-Acceptor Organic Solvents at 298.15 K

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Abstract—Enthalpies of dissolution at infinite dilution (298.15 K) of aniline, *N*-methylaniline, and *N,N*-dimethylaniline in a series of proton-acceptor solvents of different classes of compounds have been measured. The solvation enthalpies have been determined, and its relationship with the anilines structure has been analyzed. Enthalpy of hydrogen bonding in the complexes of aniline (1 : 2) and *N*-methylaniline (1 : 1) with the solvents has been calculated. In the case of aniline complexes, negative cooperativity of hydrogen bonding has been revealed, the effect enhancing with increasing the solvent proton-acceptor ability.

Keywords: aniline, solution enthalpy, solvation, hydrogen bond, cooperativity

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Physicochemical properties and reactivity of organic compounds essentially change on going from the gas phase in the solution [1]. The difference is due to various intermolecular interactions formed in the condensed phase. The intermolecular interactions affect equilibrium, rate, and mechanism of the chemical and physical processes. Hydrogen bonds are among the most important types of the interactions occurring in the solutions of organic compounds [2]. Hydrogen bonds are often cooperative (non-additive) meaning that the strength of the sequentially formed hydrogen bonds depends on the number and type of the already existing hydrogen bonds [3, 4]. The cooperative effects can strengthen (positive cooperativity) as well as weaken (negative cooperativity) the hydrogen bonds in the multicomponent complexes as compared with the 1 : 1 complex. The cooperative effects are especially important in the cases of supramolecular and biological systems [5, 6] as well as in solvents self-associated via hydrogen bonds [7, 8].

Modern studies have been mainly devoted to theoretical exploration of hydrogen bonding cooperativity in the gas phase [9–12]. In particular, a series of papers [9–11] has discussed the cooperativity in the model biological systems. The influence of size and structure of amide complexes on the derived energy of the cooperative hydrogen bonds has been elucidated [10, 11]. At the same time, experimental studies of estimating quantitative parameters of cooperative hydrogen bonds in the condensed phase have been scarce. Most of the published researches have been carried out using IR spectroscopy in a solid inert gas matrix at very low temperature [13–16]. Experimental results on the cooperative effects in the solution at standard conditions have been reported in [17–20]. Basing on the changes of the frequency of IR stretching vibrations and NMR chemical shifts of the protons, strengthening of hydrogen bonds in the multicomponent complexes of NH- and OH-donors with proton-acceptor organic compounds has been measured. Further studies of IR spectra [21–24] have quantified the cooperativity parameters in the cases of intermolecular complexes as functions both of the solvent proton-acceptor and proton-donor abilities and of the steric effects.

Calorimetry methods have been applied to studies of hydrogen bonds cooperativity as well. Approaches to determine the enthalpy of cooperative hydrogen bonds in the multicomponent complexes from experimental data on enthalpy of solution have been suggested and validated in [7, 25–27]. In particular, in

Table 1. Enthalpy of solution of aniline ($\Delta_{soln}H^{I/S}$), *N*-methylaniline ($\Delta_{soln}H^{II/S}$), and *N,N*-dimethylaniline ($\Delta_{soln}H^{III/S}$) in the proton-acceptor solvents (kJ/mol, 298.15 K)

Solvent no.	Solvent (S)	$\Delta_{soln}H^{I/S}$	$\Delta_{soln}H^{II/S}$	$\Delta_{soln}H^{III/S}$
1	Acetonitrile	0.00[a]	2.12±0.01[b]	3.20±0.02[b]
2	Acetone	–5.44[a]	–2.10±0.14[b]	1.14±0.01[b]
3	*N,N*-Dimethylformamide	–10.45±0.05[b] (–11.2)[c]	–5.55±0.02[b] (–5.3)[d]	0.66±0.02[b] (0.59)[d]
4	Dimethylsulfoxide	–9.55±0.01[b] (–10.9)[c]	–3.40±0.01[b] (–3.4)[e]	3.90±0.01[b]
5	Dibutyl ether	–1.75±0.05[b] (2.92)[c]	–0.50±0.02[b] (1.21)[e]	2.19±0.08[b]
6	1,4-Dioxane	–4.6[a]	–2.04±0.08[f] (–2.1)[e]	0.79±0.07[b]
7	Diethyl ether	–4.01±0.14[b]	–2.51±0.11[b]	1.80±0.12[b]
8	2-Methylpyridine	–8.79±0.02[b]	–6.00±0.03[b]	–0.34±0.07[b]
9	3-Methylpyridine	–8.50±0.05[b]	–6.25±0.12[b]	–0.37±0.06[b]
10	4-Methylpyridine	–8.72±0.13[b]	–6.36±0.25[b]	–0.41±0.01[b]
11	Pyridine	–7.4[d]	–5.00±0.03[b] (–4.3)[d]	0.13[d]
12	Propionitrile	–2.79±0.07[b]	–0.70±0.06[b]	0.93±0.01[b]
13	Tetrahydrofuran	–7.34±0.11[b]	–5.00±0.03[b]	–1.12±0.03[b]
14	Ethyl acetate	–2.92±0.02[b] (–3.5)[c] (–3.2)[d]	–1.11±0.13[b] (–1.4)[e] (–1.1)[d]	1.00±0.01[b] (1.0)[d]

[a] Data from [31]. [b] Determined in this work. [c] Data from [32]. [d] Data from [28]. [e] Data from [33]. [f] Data from [34].

the cases of aliphatic alcohols complexes with pyridine derivatives the value of cooperative effect is nearly constant disregarding the components structure, whereas in the cases of the complexes with tertiary aliphatic amines the cooperativity decreases with increasing of alkyl substituents in amines and alcohols [27].

In this work we applied the solution calorimetry in order to determine the negatively cooperative hydrogen bonds formation; aniline and its *N*-methyl derivatives were used as the model compounds forming the complexes. Aniline was capable of the 1 : 2 complexes formation with the proton-acceptor molecules. By an example of three bases it was demonstrated that half enthalpy of aniline hydrogen bonding with two base molecules (the 1 : 2 complex formation) was lower as compared with enthalpy of aniline hydrogen bonding with a single base molecule (the 1 : 1 complex) [28–30]. However, enthalpies of the hydrogen bond formation between aniline or its *N*-methyl derivatives and the proton acceptors as determined in different studies [28–30] significantly varied.

We determined enthalpy of solution (298.15 K) of aniline **I**, *N*-methylaniline **II**, and *N,N*-dimethyl-aniline **III** in 14 proton-acceptor solvents representing various classes of organic compounds. The corresponding enthalpies of solvation and of hydrogen bonding in different anilines complexes were derived from those data, and the solvent effect on the negative cooperativity was analyzed.

The solvents used did not show any proton-donating properties, and their proton-acceptor ability was significantly different. The amines solution enthalpies at infinite dilution are listed in Table 1. The experimental data are in good agreement with the available reference data, the only exception being the $\Delta_{soln}H^{I/S}$ value in the case of S = dibutyl ether. Data in Table 1 demonstrated that the $\Delta_{soln}H^{I/S}$ and $\Delta_{soln}H^{II/S}$ values were negative for nearly all the solvents, whereas the majority of the $\Delta_{soln}H^{III/S}$ values were positive.

The solution enthalpy reflects the heat effect corresponding to transfer of 1 mole of the solute to the infinitely diluted solution (298.15 K and 1 bar) starting from the pure solute standard state. The solution enthalpy could be represented as a sum of three energy terms corresponding to the solute–solute bonds ruptur (endothermic process), formation of the cavity in the

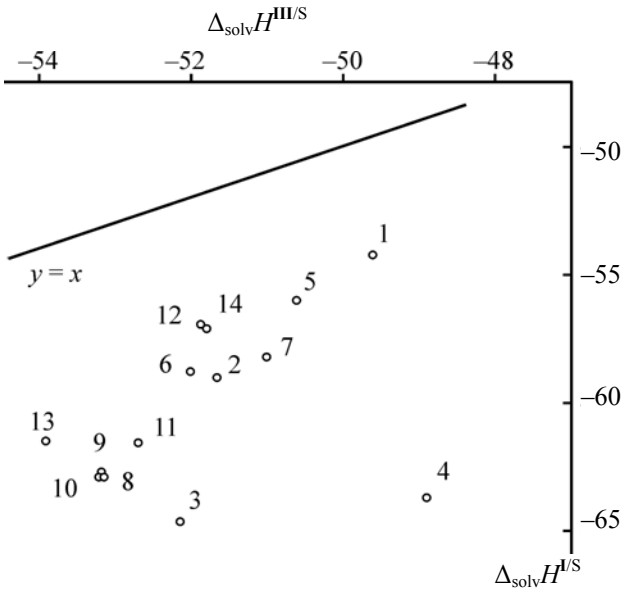


Fig. 1. Enthalpy of *N,N*-dimethylaniline solvation in the proton-acceptor solvents at 298.15 K ($\Delta_{solv}H^{III/S}$) as compared with that of aniline ($\Delta_{solv}H^{I/S}$). Data point numbers correspond to numbers of the solvents in Table 1.

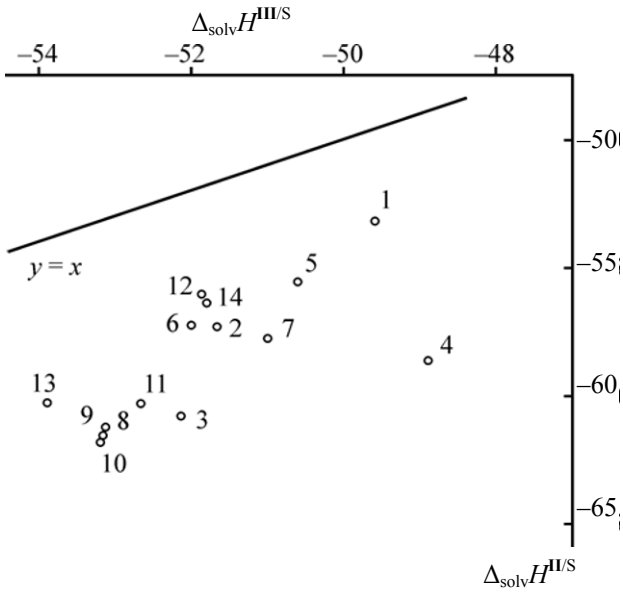


Fig. 2. Enthalpy of *N,N*-dimethylaniline solvation in the proton-acceptor solvents at 298.15 K ($\Delta_{solv}H^{III/S}$) as compared with that of *N*-methylaniline ($\Delta_{solv}H^{II/S}$). Data point numbers correspond to numbers of the solvents in Table 1.

solvent (in other words, the breaking of the solvent–solvent bonds, endothermic process), and the formation of the solute–solvent bonds (exothermic process). Hence, the collected experimental data showed that in the cases of aniline and *N*-methylaniline the solute–solvent intermolecular bonds were stronger than the sum of the solute–solute and the solvent–solvent bonds, the trend is being opposite in the case of *N,N*-dimethylaniline solutions.

The solvation enthalpy could be used as a measure of total energy of solute–solvent intermolecular interactions. The solvation enthalpy is defined as heat effect of transfer of 1 mol of the solute into the solution (298.15 K and 1 bar) starting from the ideal gas state. The solvation enthalpy is related to the solution enthalpy as expressed by Eq. (1).

$$\Delta_{solv}H^{A/S} = \Delta_{soln}H^{A/S} - \Delta_{vap}H^{A}, \quad (1)$$

where $\Delta_{vap}H^{A}$ is the solute enthalpy of vaporization at 298.15 K.

Taking into account vaporization enthalpies of the studied amines (54.2, **I**; 55.3, **II**; and 52.8, **III** kJ/mol [35]) and the measured solution enthalpies (Table 1), we calculated the corresponding solvation enthalpies $\Delta_{solv}H^{A/S}$ using Eq. (1). Figures 1 and 2 present comparison of *N,N*-dimethylaniline solvation enthalpies $\Delta_{solv}H^{III/S}$ with those of aniline $\Delta_{solv}H^{I/S}$ and *N*-methyl-aniline $\Delta_{solv}H^{II/S}$; the solid lines in the plots represent the $y = x$ equation.

From Figs. 1 and 2 it is seen that solvation of aniline and *N*-methylaniline in all probed proton-acceptor solvents was more exothermic than that of *N,N*-dimethylaniline. The solvation enthalpy of amine A in solvent S could be conventionally expressed as a sum of enthalpies of the non-specific solvation $\Delta_{solv(n/sp)}H^{A/S}$ (reflecting the van der Waals interactions in the solution) and of the hydrogen bonds formation between the solute and the solvent $\Delta_{HB}H^{A/S}$, see Eq. (2). The more negative values of $\Delta_{solv}H^{I/S}$ and $\Delta_{solv}H^{II/S}$ as compared with the $\Delta_{solv}H^{III/S}$ values were due to the presence of protons capable of hydrogen bonding with the proton-acceptor solvents in amines **I** and **II**.

$$\Delta_{solv}H^{A/S} = \Delta_{solv(n/sp)}H^{A/S} + \Delta_{HB}H^{A/S}. \quad (2)$$

We further determined the enthalpies of hydrogen bonds formation by the studied anilines. Using the previously developed approach [33] based on Eq. (3). The method was successfully used in [7, 25–27, 33] to determine a number of hydrogen bonding enthalpies in certain solute–solvent systems.

$$\Delta_{HB}H^{A/S} = \Delta_{soln}H^{A/S} - (\delta_{cav}h^{S} - \delta_{cav}h^{C_6H_{12}})V_X^{A} - \Delta_{soln}H^{A/C_6H_{12}} - (a_R + b_R\sqrt{\delta}_{cav}h^{S})[(\Delta_{soln}H^{A/R} - \Delta_{soln}H^{A/C_6H_{12}}) - (\delta_{cav}h^{R} - \delta_{cav}h^{C_6H_{12}})V_X^{A}], \quad (3)$$

Table 2. Characteristic volume (V_X^A) and solution enthalpies in the reference solvents[a] ($\Delta_{soln}H^{A/R}$) and in cyclohexane ($\Delta_{soln}H^{A/C_6H_{12}}$) of the studied amines at 298.15 K

Amine A	$V_X^A \times 10^{-2}$, cm^3/mol	$\Delta_{soln}H^{A/R}$, kJ/mol	$\Delta_{soln}H^{A/C_6H_{12}}$, kJ/mol
Aniline **I**	0.8160	8.66±0.04[b]	15.56±0.54[b]
N-Methylaniline **II**	0.9571	5.61±0.00[b]	11.59±0.17[b]
N,N-Dimethylaniline **III**	1.0980	0.66±0.50[c]	6.44±0.12[b]

[a] The following solvents were used as reference ones: tetrachloromethane (A = aniline and *N*-methylaniline) and benzene (A = *N,N*-dimethylaniline). [b] Data from [33]. [c] Determined in this work.

Table 3. Specific relative enthalpy of cavity formation for proton-acceptor solvents ($\delta_{cav}h^S$) and enthalpy of hydrogen bonds formation between the solvents and aniline ($\Delta_{HB}H^{I/S}$), *N*-methylaniline ($\Delta_{HB}H^{II/S}$), and *N,N*-dimethylaniline ($\Delta_{HB}H^{III/S}$) at 298.15 K

Solvent no.	Solvent (S)	$\delta_{cav}h^S \times 10^2$, kJ/cm^3	$\Delta_{HB}H^{I/S}$, kJ/mol	$\Delta_{HB}H^{II/S}$, kJ/mol	$\Delta_{HB}H^{III/S}$, kJ/mol	β[f], kJ/mol
1	Acetonitrile	10.66[a]	–6.1[a]	–3.3	0.7	0.40
2	Acetone	7.65[a]	–11.3[a]	–6.6	0.0	0.48
3	*N,N*-Dimethylformamide	8.62[a]	–16.3 (–20.2)[c] (–16.7)[d]	–10.3 (–11.0)[c] (–14.6)[e]	–0.9	0.69
4	Dimethylsulfoxide	13.87[a]	–16.1 (–19.3)[d]	–10.1 (–16.7)[e]	–0.5	0.76
5	Dibutyl ether	0.53[a]	–10.8	–6.2 (–4.4)[a]	1.7	0.46
6	1,4-Dioxane	7.57[a]	–10.4[a]	–6.5[a]	–0.3	0.37
7	Diethyl ether	1.59[a]	–11.6	–7.1	1.7	0.47
8	2-Methylpyridine	4.66[b]	–15.0	–10.0	–0.3	0.72
9	3-Methylpyridine	4.98[b]	–14.5	–10.3	–0.5	0.68
10	4-Methylpyridine	4.58[b]	–14.8	–10.4	–0.5	0.67
11	Pyridine	6.66[a]	–13.2[a] (–16.6)[c]	–9.3 (–9.6)[c]	–0.7	0.64
12	Propionitrile	7.32	–8.6	–5.1	0.0	0.37
13	Tetrahydrofuran	3.28[a]	–13.9	–9.0 (–12.1)[e]	–1.0	0.55
14	Ethyl acetate	5.98[a]	–8.8 (–13.3)[c]	–5.2[a] (–7.2)[c]	0.6	0.45

[a] Data from [33]. [b] Data from [37]. [c] Data from [28]. [d] Data from [29]. [e] Data from [30].

where $\Delta_{soln}H^{A/S}$, $\Delta_{soln}H^{A/C_6H_{12}}$, and $\Delta_{soln}H^{A/R}$ are enthalpies of dissolution of compound A in the studied solvent S, cyclohexane, and the reference solvent R, respectively; $\delta_{cav}h^S$, $\delta_{cav}h^{C_6H_{12}}$, and $\delta_{cav}h^R$ are the specific relative enthalpies of cavity formation in the same solvents [33]; V_X^A is the characteristic volume of the solute calculated using the McGowan additive scheme [36]; a_R and b_R are empirical parameters determined for the reference solvent R by means of regression analysis. The solvent to be used as reference should not form hydrogen bonds with the solute; accounting for that, tetrachloromethane is often used as reference solvent

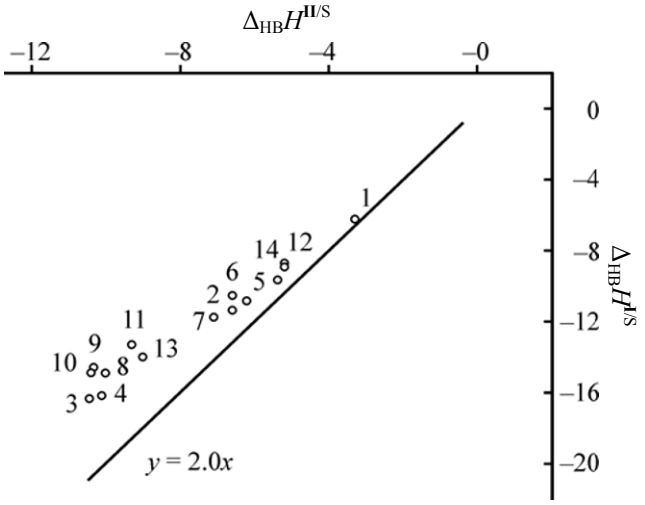


Fig. 3. Enthalpy of hydrogen bonding of *N*-methylaniline with the proton-acceptor solvents at 298.15 K ($\Delta_{HB}H^{II/S}$) as compared with that of aniline ($\Delta_{HB}H^{I/S}$). Data point numbers correspond to numbers of the solvents in Table 3.

when studying the proton-donor compounds (a_R 0.34, b_R 0.61), whereas benzene (a_R 0.20, b_R 0.38) serves as reference in the case of proton-acceptor solutes.

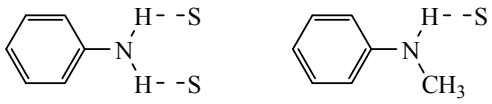
The anilines parameters required for calculation of the hydrogen bonding enthalpy are collected in Table 2.

Specific relative enthalpies of cavity formation of the studied solvents are listed in Table 3. The corresponding values for cyclohexane (1.42×10^2 kJ/cm^3), tetrachloromethane (1.91×10^2 kJ/cm^3), and benzene (5.02×10^2 kJ/cm^3) were found in [33]. Tetrachloromethane was used as reference solvent for aniline and *N*-methylaniline, benzene served as reference solvent for *N,N*-dimethylaniline.

The enthalpies of hydrogen bond formation between the amines **I**–**III** and the studied proton-acceptor solvents calculated using Eq. (3) are collected in Table 3 as well.

The calculated hydrogen bonding enthalpies were significantly different for the studied amines. In particular, the $\Delta_{HB}H^{III/S}$ values were close to zero in the cases of all studied solvents (within the method accuracy of about 1.5 kJ/mol), as *N,N*-dimethylaniline could not act as proton donor. In the cases of the other two anilines, hydrogen bonding enthalpy depended on the solvent. The last column in Table 3 shows the values of parameter β quantifying the proton-acceptor ability of organic compounds [38]. The strongest hydrogen bonds were formed by aniline or *N*-methylaniline with *N,N*-dimethylformamide, dimethylsulfoxide, and the pyridines (Table 3). Noteworthily, those solvents showed the highest values of parameter β. Most of the enthalpies determined in this work were in good agreement with the available reference data (collected in Table 3 for comparison).

Absolute values of hydrogen bonding enthalpy were higher in the case of aniline than those in the case of *N*-methylaniline (Table 3), because aniline formed the 1 : 2 complexes (**A**) upon dissolution in the proton-acceptor solvents, whereas *N*-methylaniline could only form the 1 : 1 complexes (**B**).



$\Delta_{HB}H^{I/S}$ $\Delta_{HB}H^{II/S}$

A **B**

Figure 3 demonstrates the comparison of hydrogen bonding enthalpies in the cases of *N*-methylaniline ($\Delta_{HB}H^{II/S}$) and aniline ($\Delta_{HB}H^{I/S}$) and the studied solvents. The solid line in Fig. 3 represents the $y = 2x$ equation. Deviation of the experimental data from the theoretical dependence reflected the negative cooperativity of hydrogen bonding in the course of the 1 : 2 complexes formation. In other words, the two hydrogen bonds in the 1 : 2 complexes were weaker than the pair of the single hydrogen bonds in the corresponding 1 : 1 complexes [see Eq. (4)]. Data in Table 3 and Fig. 3 revealed that the negative cooperativity increased linearly with the solvent proton-acceptor ability. Hence, for the stronger proton acceptors the total enthalpy of the 1 : 2 complexes formation could be comparable to those in the case of the 1 : 1 complexes, containing only one hydrogen bond.

$$(-\Delta_{HB}H^{I/S}) < (-2\Delta_{HB}H^{II/S}). \quad (4)$$

To conclude, we demonstrated that the cooperativity effect significantly influenced the determined thermodynamic parameters, and it should be accounted for when discussing the multicomponent systems.

EXPERIMENTAL

Aniline, *N*-methylaniline, and *N,N*-dimethylaniline (98%, Across Organics) were purified by vacuum distillation over calcium hydride. All the solvents used were commercially available with purity of >98%. Prior to the measurements, the solvents were purified and dried as described elsewhere [39]. Content of the impurities in the studied compounds were monitored

using the KONIK 5000 gas chromatograph equipped with the flame ionization detector. Content of water was determined via the Fischer method using the C20 Mettler Toledo titrator.

Dissolution enthalpies were measured at 298.15 K using the pseudo adiabatic solution calorimeter as described previously [27]. The Dewar vessel (the solvent volume of 110 mL and the solute mass of 0.03–0.06 g) was used as the calorimetric cell. The calorimetric measurement validity was verified by determination of enthalpy of 1-propanol dissolution in water; the measured value (10.08 ± 0.01 kJ/mol at 298.15 K and *m* 0.0238 mol/kg) coincided with the reference value for the tested system (10.10 ± 0.02 kJ/mol [40]).

All the determined dissolution enthalpies corresponded to the infinite dilution as confirmed by the absence of concentration effects in the used concentration ranges.

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