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Hydrogen Bonding of Aliphatic and Aromatic Amines in Aqueous Solution: Thermochemistry of Solvation

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Abstract—Thermochemistry of hydration of the aliphatic and aromatic amines was studied. Enthalpies of solution at infinite dilution of amines in water were measured using the method of solution calorimetry. A procedure of taking into account the ionization and non-specific hydration of amines in aqueous media was carried out. A method for estimating the enthalpy of hydrogen bonding of amines in aqueous solutions was suggested on the basis of a comparative analysis of the solvation enthalpies of the solutes in water and methanol. The efficiency of this method is confirmed by evaluating the hydrophobic effect enthalpy.

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Water plays an important role in various biological, technological and chemical processes [1]. Water is a liquid whose molecules are associated through hydrogen bonds and form complicated complexes of different structure and composition. The self-association of water molecules is a key factor determining its physical and chemical properties [2].

Water as a solvent can significantly affect the reactivity of an organic compound forming hydrogen bonds with its molecules [3]. Thus, the basicity (acidity) order of organic compounds in a series of homologues can vary significantly going from a gas phase to the aqueous solution [4, 5]. For example, the basicity of methylamines in the gas increases with successive increase in the number of alkyl substituents in the molecule [6], whereas in water it is changed in a series of $Me_2NH > MeNH_2 > Me_3N > NH_3$ [7]. Many amines and nitrogen heterocycles are fragments of biologically active substances. The nitrogen atom, being a part of such organic molecules, is a strong proton-acceptor fragment, which is involved in the non-covalent binding with the active sites of receptors and enzymes. In the aqueous solution the substrate–enzyme complexes stability depends on the hydrogen bonding energy of the reacting molecules with the water molecules. Therefore, the determination of the thermodynamic functions of hydrogen bonding of amines with water is an actual task.

Previously the hydrogen bonding of water molecules with amines (A) has been actively studied in the gas phase, in inert solvents (carbon tetrachloride, benzene, etc.) or in the pure base. Some authors used various spectroscopic [8–10] and thermochemical [11–13] methods, as well as theoretical calculations [14, 15]. However, experimental data on the energy of hydrogen bonding of amines in the pure water remains quite scanty. This is due to the fact that they cannot be determined by spectroscopic methods. A more suitable approach to the study of the energy of hydrogen bonding of solutes in water is based on the analysis of the thermodynamic functions of solvation and dissolution. The energy of hydrogen bonding of amines with water obtained in the framework of this approach differs from the energy of the hydrogen bond formation in equimolar complexes (H–O–H···A) in an inert environment [16, 17]. This difference is due, firstly, to the fact that amines dissolved in water form multiparticle complexes with the water associates, in which hydrogen bonds are stronger due to cooperative interaction [17]. Secondly, since almost all water molecules participate in the formation of hydrogen bonds, the dissolution of amines in water can cause rupture of a part of the water–water interactions [13].

In [17] a method for estimating the Gibbs energy of hydrogen bonding of amines in pure water has been proposed. The method is based on the general dependence of the Gibbs energy of hydrophobic effect on the volume of the dissolved molecules. This method allows the estimation of the Gibbs energy of hydrogen bonding between the dissolved molecules and the liquid water. In this paper we propose a method for the evaluation of the hydrogen bonding enthalpy of amines in aqueous solutions based on the analysis of the enthalpies of solvation of solutes in water and methanol.

To study the hydrogen bonding we used a method of the thermochemistry of solvation. The solvation enthalpy of a solute A in a solvent S was calculated from the experimentally measured values in accordance with Eq. (1):

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

where $\Delta_{\text{soln}}H^{\text{A/S}}$ is the solution enthalpy of A in the solvent S at the infinite dilution, $\Delta_{\text{vap}}H^{\text{A}}$ is the enthalpy of vaporization of the solute A. The value of $\Delta_{\text{solv}}H^{\text{A/S}}$ reflects the energy of intermolecular interactions in the solution. It can be expressed as a sum of the enthalpies of nonspecific solvation $\Delta_{\text{solv(nonsp)}}H^{\text{A/S}}$ and the specific interaction $\Delta_{\text{int(sp)}}H^{\text{A/S}}$ of the solute in the solvent:

$$\Delta_{\text{solv}}H^{\text{A/S}} = \Delta_{\text{solv(nonsp)}}H^{\text{A/S}} + \Delta_{\text{int(sp)}}H^{\text{A/S}}. \quad (2)$$

The enthalpy of specific interaction $\Delta_{\text{int(sp)}}H^{\text{A/S}}$ presents the enthalpy of the localized donor–acceptor interaction between the solute and the solvent, including hydrogen bonding. In the case of associated solvents, such as water, the value of $\Delta_{\text{int(sp)}}H^{\text{A/S}}$ may include two components: the enthalpy of breaking some solvent–solvent hydrogen bonds (reorganization) and the enthalpy of hydrogen bonding of solute with the solvent associates. In [18] an equation for calculating the enthalpy of nonspecific solvation of the solute A in solvent S was proposed:

$$\begin{aligned}\Delta_{\text{solv(nonsp)}}H^{\text{A/S}} &= (\delta_{\text{cav}}h^{\text{S}} - \delta_{\text{cav}}h^{\text{C}_6\text{H}_{12}})V_{\text{X}}^{\text{A}} + \Delta_{\text{solv}}H^{\text{A/C}_6\text{H}_{12}} \\ &+ (a_{\text{R}} + b_{\text{R}}\sqrt{\delta_{\text{cav}}h^{\text{S}}})[(\Delta_{\text{solv}}H^{\text{A/R}} - \Delta_{\text{solv}}H^{\text{A/C}_6\text{H}_{12}}) \\ &- (\delta_{\text{cav}}h^{\text{R}} - \delta_{\text{cav}}h^{\text{C}_6\text{H}_{12}})V_{\text{X}}^{\text{A}}], \quad (3)\end{aligned}$$

where $\Delta_{\text{solv}}H^{\text{A/C}_6\text{H}_{12}}$ and $\Delta_{\text{solv}}H^{\text{A/R}}$ are the solvation enthalpies of A in cyclohexane and in a reference solvent R, which is not capable to specific interaction with the solute, respectively; V_{X}^{A} is the McGowan's characteristic volume [19]; $\delta_{\text{cav}}h^{\text{S}}$, $\delta_{\text{cav}}h^{\text{R}}$ and $\delta_{\text{cav}}h^{\text{C}_6\text{H}_{12}}$ are the specific relative enthalpies of the cavity formation in the solvent S, R, and cyclohexane. The value of $\delta_{\text{cav}}h^{\text{S}}$ characterizes the ability of solvent to non-specific interactions. These values for various solvents can be found in [18].

Joint application of Eqs. (1) and (3), and using the experimental data on the enthalpies of dissolution in the studied systems makes it possible to estimate the enthalpy of the hydrogen bonding.

The determination of the energy of hydrogen bonding of amines in water is rather complicated due to the necessity of the correct identification of two additional contributions to the thermodynamic functions of hydration: ionization of amines $\Delta_{\text{ion}}H^{\text{A}}$ and the hydrophobic effect $\Delta_{\text{h.e.}}H^{\text{A}}$. The latter contribution is manifested in the anomalous values of the thermodynamic functions of dissolution in aqueous solutions [20].

Taking into account the additional contributions, Eq. (2) for aqueous solutions of amines is transformed into Eq. (4):

$$\begin{aligned}\Delta_{\text{hydr}}H^{\text{A/H}_2\text{O}} &= \Delta_{\text{hydr(nonsp)}}H^{\text{A/H}_2\text{O}} + \Delta_{\text{h.e.}}H^{\text{A}} \\ &+ \Delta_{\text{int(sp)}}H^{\text{A/H}_2\text{O}} + \Delta_{\text{ion}}H^{\text{A}}. \quad (4)\end{aligned}$$

The ionization of amines in aqueous solution can be described by the following scheme: $\text{A} + \text{H}_2\text{O} = \text{AH}^+ + \text{OH}^-$.

The extent of ionization of amines depends on their structure. The extent of ionization of primary aliphatic amines may reach 10–20%, of secondary amines, 30% [21]. At the same time, for pyridines it is 0.1% [22], so the $\Delta_{\text{ion}}H^{\text{A}}$ contribution in the latter case may be ignored.

The term $\Delta_{\text{h.e}}H^{\text{A}}$ reflects the peculiarities of liquid water compared to other solvents. It was shown in [23, 24] that the enthalpy of hydrophobic effect of *n*-alkanes is equal to -10.7 ± 1.5 kJ mol^{-1} and is independent of the length of the alkyl radical. For aromatic hydrocarbons the enthalpy of the hydrophobic effect is positive [23, 24], and it increases with increasing volume of the molecule.

In order to estimate the hydrogen bonding enthalpy of amines in water it is necessary to determine correctly the values in Eq. (4).

In this paper we studied the thermochemistry of solvation of amines in aqueous solutions. The enthalpy of solution of amines in water at the infinite dilution was measured experimentally, a part of the data was taken from the literature, when several different values were published we preferred the values of the more recent works. The enthalpies of amines dissolution in water are listed in Table 1. Using the experimentally measured values, we calculated the hydration enthalpies with Eq. (1). They also are listed in Table 1. The vaporization enthalpies were taken from [25].

Table 1. Enthalpies of solution of amines in water at 298.15 K, vaporization of amines, hydration and ionization of amines in aqueous solution (kJ mol^{-1})

Base (A)	$\Delta_{soln(exp)}H^{A/H_2O}$	$\Delta_{vap}H^{A}$	$\Delta_{hydr}H^{A}$	$\Delta_{prot}H^{A\,a}$
n-Butylamine	–23.46 [26]	35.7	–59.2	58.51 [28]
sec-Butylamine	–24.50±0.35	32.6	–57.1	58.65 [22]
tert-Butylamine	–28.95 [26]	30.5	–59.5	60.00 [22]
n-Hexylamine	–21.67±0.24	45.0	–66.7	58.97 [29]
Cyclohexylamine	–23.73±0.13	42.8	–66.5	59.66 [29]
Diethylamine	–28.29 [27]	32.7	–61.0	53.21 [22]
Piperidine	–26.14 [26]	–	–	53.36 [22]
Pyridine	–1.94 [26]	40.2	–42.1	b
2-Methylpyridine	–7.80 [26]	42.5	–50.3	b
3-Methylpyridine	–5.75 [26]	44.6	–50.4	b

[a] The enthalpy of the process $AH^+ \rightleftarrows A + H^+$. [b] The degree of ionization of pyridines < 0.1%.

To determine the energy of hydrogen bonding of amines in water according to Eq. (4) it is necessary to estimate correctly the additional contributions to the amine hydration enthalpy. First we assessed the contribution due to the process of the amine ionization at the dissolution in water. We took into account two processes: the proton cleavage from water molecule and the ionization of amine to form ammonium cation. Therewith two processes were taken into account: the elimination of the proton from the water molecule and the amine ionization to give ammonium cation. The enthalpy of the amine ionization was subtracted from the experimentally measured solution enthalpy. The fraction of amine molecules in the ionized form (AH^+) α was taken into account:

$$\Delta_{ion}H^{A} = \alpha(\Delta_{prot}H^{A} + \Delta_{w}H^{A}).$$

The enthalpy of water ionization ($\Delta_{w}H^{A}$ = –55.8 kJ mol^{-1}) is taken from [30]. The enthalpy of hydration of pyridine does not contain the ionization contribution [21, 22]. Therefore the $\Delta_{soln}H^{A/H_2O}$ values for pyridines were used in the subsequent calculations of energy of hydrogen bonding without the correction for the ionization.

The next contribution in Eq. (4), which should be estimated to determine the enthalpy of hydrogen bonding of amine in water, is the enthalpy of nonspecific hydration. The value of $\Delta_{hydr(nonsp)}H^{A/H_2O}$ can be calculated using various methods [31]. In this paper we use Eq. (3). The required enthalpies of the amines dissolution in cyclohexane ($\delta_{cav}h^{C_6H_{12}}$ = 1.42×10^2 kJ cm^{-3}) and in the reference solvent benzene ($\delta_{cav}h^{C_6H_6}$ = 5.02×10^2 kJ cm^{-3}, a_R = 0.20, b_R = 0.38) are listed in Table 2. Table 2 contains also the characteristic molecular volumes of amines by McGowan. The value for water, $\delta_{cav}h^{H_2O}$ = (9.5±1.0)× 10^2 kJ cm^{-3}, was taken from [24]. The calculated enthalpies of nonspecific hydration are shown in Table 2. The last column of Table 2 lists the differences of the enthalpies of hydration and non-specific hydration of the studied amines. These values are the sums of the enthalpies of specific interaction of amines in water and the enthalpies of hydrophobic effect of the amines.

The question arises: how to separate these two contributions and estimate the unknown enthalpy of specific interaction of amines in water corresponding to the process of hydrogen bonding? The enthalpy of solvation in methanol and the other aliphatic alcohols is known not to include the solvophobic effect. Therefore, we can calculate the enthalpy of hydrogen bonding in the alcohol with the Eqs. (2) and (3). Methanol contains both a proton-donor and a proton-acceptor sites, its molecule is small in volume, and it is a close structural analog of water. Therefore, we decided to compare the energy of hydrogen bonding in water environment with the specific interaction enthalpy in methanol.

Comparing the enthalpies of self-association of water (–14.0±1.0 kJ mol^{-1} [33, 34]) and methanol (–15.1 kJ mol^{-1} [35]) per one OH group, one can see that they are of close values. The enthalpy of hydrogen bonding of water in methanol calculated with Eqs. (2) and (3) is equal to –14.6 kJ mol^{-1}, which also is consistent with these data. The published data on the

Table 2. The characteristic molecular volumes of amines (cm^3 mol^{-1}), enthalpies of solution in cyclohexane and benzene at 298.15 K, the sum of the enthalpies of specific interaction and hydrophobic effect of amines in water (kJ mol^{-1})

Base (A)	$V_x^A\times10^{-2}$	$\Delta_{soln}H^{A/C_6H_{12}}$	$\Delta_{soln}H^{A/C_6H_6}$	$\Delta_{hydr(nonsp)}H^{A/H_2O}$	$\Delta_{int(sp)}H^{A/H_2O} + \Delta_{h.e.}H^A$
n-Butylamine	0.7720	6.48±0.05	2.87±0.10	–31.5	–27.7
sec-Butylamine	0.7720	5.95±0.14	1.55±0.07	–30.0	–27.1
tert-Butylamine	0.7720	5.15±0.12	1.27±0.03	–27.9	–31.6
n-Hexylamine	1.0538	6.41±0.09	2.30±0.03	–40.1	–26.6
Cyclohexylamine	0.9452	4.98±0.03	2.05±0.03	–38.4	–28.1
Diethylamine	0.7720	3.50±0.06	0.87±0.03	–30.4	–30.6
Piperidine	0.8043	4.50±0.09	1.80±0.04	–	–28.6 [a]
Pyridine	0.6753	8.20±0.2 [32]	0.0±0.0 [32]	–41.0	–1.1
2-Methylpyridine	0.8162	6.57±0.04 [32]	–0.54±0.08 [32]	–43.1	–7.2
3-Methylpyridine	0.8162	8.44±0.20 [32]	0.44±0.05 [32]	–44.7	–5.7

[a] The value of $\Delta_{int(sp)}H^{A/H_2O} + \Delta_{h.e.}H^A$ for piperidine is calculated from the enthalpies of dissolution.

enthalpies of complexation of water or methanol with a proton-acceptor in the environment of pure base or inert solvent are close to each other [36]. For example, the enthalpy of formation of the pyridine–water complex is –17.1 kJ mol^{-1} [8], the hydrogen bonding enthalpy of methanol–pyridine complex is –16.3 kJ mol^{-1} [36].

$$1/2\Delta_{HB}H^{H_2O/H_2O} \approx \Delta_{HB}H^{CH_3OH/CH_3OH} \approx \Delta_{HB}H^{H_2O/CH_3OH}. \quad (5)$$

The equality (5) as well as similarity of the published data on the enthalpies of complexation of proton-acceptors with either water, or methanol give a reason to assume that the enthalpy of specific interaction of proton-acceptors in methanol and water also are close to each other. If this is correct, then the value of $\Delta_{int(sp)}H^{A/H_2O}$ can be estimated from the data for methanol. This approach requires additional evidence.

Proceeding from the Eq. (4), the enthalpy of hydrophobic effect of amines can be calculated as follows:

$$\Delta_{h.e.}H^A = \Delta_{hydr}H^{A/H_2O} - \Delta_{hydr(nonsp)}H^{A/H_2O} - \Delta_{int(sp)}H^{A/H_2O} - \Delta_{ion}H^A. \quad (6)$$

If the assumption about equality of the enthalpies of hydrogen bonding with water and methanol is correct, Eq. (6) can be written as Eq. (7).

$$\Delta_{h.e.}H^A = \Delta_{hydr}H^{A/H_2O} - \Delta_{hydr.(nonsp)}H^{A/H_2O} - \Delta_{int(sp)}H^{A/CH_3OH} + \Delta_{ion}H^{A/CH_3OH}. \quad (7)$$

The enthalpy of hydrophobic effect of amine calculated with Eq. (6) should be negative for the amines with aliphatic substituent, and positive in the case of aromatic structure of the molecule.

Table 3 lists the enthalpies of solution of amines in methanol. To calculate the enthalpies of specific interaction of amines in methanol by Eqs. (1), (2) and (3) we used the enthalpies of dissolution of amines in benzene and cyclohexane (Table 2), the specific relative enthalpy of cavity formation in methanol is 5.10×10^2 kJ cm^{-3} [35].

Table 3 lists the specific interaction enthalpies of amines in methanol, $\Delta_{int(sp)}^{A/CH_3OH}$. The values are negative and smaller than the enthalpies of formation of equimolar complexes in the medium of a base ($\Delta_{H\text{-}bond}^{CH_3OH\cdots A}$). For instance, the enthalpy of formation of the 3-methylpyridine complex with methanol is equal to –17.9 kJ mol^{-1} [32], whereas the enthalpy of specific interaction of 3-methylpyridine in methanol is –5.2 kJ mol^{-1} [32]. This difference is caused by the cleavage of hydrogen bonds in the methanol medium at the dissolution of the proton-acceptor. In addition, while formation of multi-particle complexes with the clusters of associated solvent the cooperative strengthening of hydrogen bonds takes place.

To determine the enthalpy of hydrophobic effect of amines, the value of $\Delta_{int(sp)}^{A/CH_3OH}$ was subtracted from the sum $\Delta_{int(sp)}^{A/H_2O}$ + $\Delta_{h.e.}H^A$ [Eq. (6)]. Table 4 lists the obtained values. The enthalpies of the hydrophobic effect of aliphatic amines are negative. On the contrary, the enthalpy of hydrophobic effect in the case of pyridine is small and positive. A different pattern is observed for the pyridine methyl derivatives. The corresponding enthalpies of hydrophobic effect are small and negative. Therewith the values of $\Delta_{h.e.}H^A$ are

Table 3. Enthalpies of solution of amines in methanol at 298.15 K and of specific interaction in methanol (kJ mol^{-1})

Base (A)	$\Delta_{soln}H^{A/CH_3OH}$	$\Delta_{int(sp)}H^{A/CH_3OH}$
n-Butylamine	–15.81±0.05	–18.4
tert-Butylamine	–18.99±0.05	–19.9
n-Hexylamine	–14.54±0.19	–16.5
Diethylamine	–16.30±0.20	–16.9
Piperidine	–13.38±0.21	–14.9
Pyridine	–4.1 [11]	–3.6 [11]
2-Methylpyridine	–7.6±0.0 [32]	–6.5 [32]
3-Methylpyridine	–5.32±0.01 [32]	–5.2 [32]

Table 4. Enthalpies of the hydrophobic effect of amines, alkanes, and aromatic compounds (kJ mol^{-1})

Compounds	$\Delta_{h.e.}H^A$
Alkanes	–10.7±1.5
Benzene	1.3
Toluene	–1.3
Aliphatic amines	–11.6±1.4
Pyridine	2.5
2-, 3-Methylpyridine	–0.7±0.1

identical for the 2- and 3-methylpyridine. We calculated the $\Delta_{h.e.}H^A$ value for toluene, whose molecule also has both aliphatic and aromatic fragments. The solution enthalpies of toluene in cyclohexane (2.94 kJ mol^{-1} [38]) and benzene (0.50 kJ mol^{-1} [39]) were used in the calculation. The estimated $\Delta_{h.e.}H^A$ of toluene is –1.3 kJ mol^{-1}. Consequently, the $\Delta_{h.e.}H^A$ value may be negative for the molecules containing both aliphatic and aromatic fragments. The $\Delta_{h.e.}H^A$ values of amines in Table 4 are compared with the enthalpy of hydrophobic effect of molecules having the same hydrocarbon skeleton but without the amino group. Table 4 shows that the enthalpies of hydrophobic effect of the bases are close to those of the *inert* counterparts. This result shows that the enthalpy of hydrogen bonding in methanol and water are close to each other. Therefore, the method we proposed for calculating the values of $\Delta_{int(sp)}^{A/H_2O}$ is correct.

Thus, the complex process of determining the energy of hydrogen bonding of amines in the aqueous solution can be reduced to a more understandable determination of the energy of specific interaction of the proton-acceptors in methanol, the structural analogue of water. The correctness of determination of the hydrogen bonding enthalpies of amines in aqueous media is confirmed by the estimation of the hydrophobic effect enthalpies. The data obtained can be used at the consideration of reactivity of dissolved compounds. However, this method seems not applicable to the case of dissolving proton-donors in water. This is due to the different contributions of the reorganization to the enthalpy of solvation of the proton-donor in methanol and water.

EXPERIMENTAL

The amines from Acros Organics used (weight fraction at least 0.98) were purified by standard methods [40]. Purity of the substances was tested chromatographically. Water was distilled twice and deionized just prior to the experiment using the purification system MilliQ (Millipore Corporation). Its purity was controlled by the pH value and conductivity at 298.15 K (5.6×10^{-6} S m^{-1} or 18.2 MΩ cm, consistent with the standard value [41]).

Calorimetric measurements were carried out at the infinite dilution in the pseudo-adiabatic calorimeter designed by the authors. A detailed description of the device is given in [32]. The limit of detection of the device is 10 μK, which corresponds to 0.005 J if the solvent is water. The reproducibility of the calorimetric data is 0.15% in the case of electrical calibrations, which corresponds to the thermal effect of 0.5–1.5 J. The calorimeter was tested by measuring the enthalpy of solution of potassium chloride in water. The experimentally obtained enthalpy of solution were averaged over 6–8 measurements. Lack of concentration dependence of the enthalpies of dissolution confirms correctness of the calorimetric experiments at infinite dilution.

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