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New method for determination of vaporization and sublimation enthalpy of aromatic compounds at 298.15 K using solution calorimetry technique and group-additivity scheme

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ABSTRACT

In this work a new method for determination of vaporization/sublimation enthalpies of aromatic compounds directly at $T = 298.15$ K was developed. This method is based on the general relationship between vaporization/sublimation enthalpy and enthalpies of solution and solvation of the studied compound in any solvent. According to this method the procedure for determination of vaporization (liquids) or sublimation (solids) enthalpy includes measurement of the solution enthalpy of the compound in a selected solvent and calculation of the solvation enthalpy for this system. A group-additivity scheme for calculation of solvation enthalpies is proposed. The solvation enthalpy of compound is estimated from the solvation enthalpy of parent aromatic or heteroaromatic compound and contributions of the substituent groups. Limiting solution enthalpies of 34 aromatic compounds (substituted benzenes, naphthalenes, biphenyls, pyrene, anthracene and pyridines) in carbon tetrachloride, benzene, acetonitrile and *N,N*-dimethylformamide were measured in the present work at 298.15 K. Vaporization/sublimation enthalpies of 78 aromatic and heteroaromatic compounds were determined directly at 298.15 K using experimentally measured solution enthalpies and predicted values of solvation enthalpies. The results are in good agreement with available literature data.

1. Introduction

Determination of thermodynamical functions of liquid–gas or solid–gas phase transitions is an important subject in chemical thermodynamics. The traditional way for evaluation of these values includes experimental studies of processes of transition from the condensed state to the gas phase usually at elevated temperatures. This procedure is not universal and has some well-known problems, which were discussed early [1,2]. Most critical of them are possible thermal instabilities of the compounds studied, significant effects of small amount of impurities on the experimental values and the ambiguity associated with extrapolation of thermochemical data from the temperature of measurements (T) to a reference temperature (298.15 K). Hence, the reliability of the vaporization/sublimation enthalpies obtained by conventional methods depends on the effect of each of these factors. In this regard, development of additional independent methods to assess phase transition enthalpies, which do not have the above-described problems, becomes a very important and useful task. First, these methods can help to resolve contradictions in existing literature data. Second, they can be applied to studies of low volatile and thermally unstable compounds, for which conventional methods are difficult or unusable. One possible way for development of such methods is application of solution calorimetry [3–8]. According to this approach vaporization (liquid solutes) or sublimation (solid solutes) enthalpies at 298.15 K can be determined from thermodynamic functions of solution ($\Delta_{soln}H^{A/S}$) and solvation ($\Delta_{solv}H^{A/S}$) of the studied compound in any solvent at 298.15 K by Eqs. (1) and (2):

$$\Delta_l^g H_m^A = \Delta_{soln}H^{A/S} - \Delta_{solv}H^{A/S} \quad (1)$$

$$\Delta_{cr}^g H_m^A = \Delta_{soln}H^{A/S} - \Delta_{solv}H^{A/S} \quad (2)$$

The enthalpy of solution required for application of Eqs. (1) and (2) can be measured experimentally by direct (solution calorimetry) or indirect (gas chromatography, solubility, etc.) techniques. The problem is how to obtain the enthalpy of solvation, because it can be measured experimentally only for gaseous compounds.

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In our previous works [3–8], a general linear dependence between enthalpies of solvation and a solutes molar refraction was found for different compounds (organic non-electrolytes from water to diphenylmercury, more than 130 compounds) in hydrocarbon solvents (*S*) particularly in cyclohexane. Thus, this dependence offers an opportunity to access enthalpies of solvation of any solute, provided that molar refractions are known and to use these values for determination of vaporization/sublimation enthalpies by Eqs. (1) and (2). However, the solution calorimetry based approach has some limitations. First, a large number of organic compounds have poor solubility in cyclohexane. Second, values for highly polar compounds are outliers from the observed linear dependence and reasons for these deviations are still not known. Correlations between enthalpy of solvation and molar refraction were also observed for a limited number of non-alkane solvents (benzene, carbon tetrachloride, etc.), but only for special series of solute compounds, for example, aromatic hydrocarbons and their halogen-derivatives [6,7]. Consequently, a more general procedure for calculation of solvation enthalpies should be developed in order to extend the applicability of the solution calorimetry approach for determination of vaporization/sublimation enthalpies.

In this work a thermochemical study of solution and solvation of aromatic compounds with different substituent groups (halogen, nitro, hydroxyl, alkyl, amino, carbonyl, etc.) in several solvents was carried out. A group-additivity scheme for calculation of solvation enthalpies was developed on the basis of experimental and literature data. According to this scheme, the enthalpy of solvation is calculated as a sum of additive contributions of fragments that construct the molecule of interest. Solvation enthalpy calculated by this manner together with the solution enthalpy at 298.15 K allows a determination of the enthalpies of vaporization and sublimation of any aromatic compound directly at 298.15 K. The method proposed in this work was tested on a number of pyridine and aromatic hydrocarbons derivatives.

2. Experimental part

2.1. Materials

Chemicals studied in this work were of commercial origin with mass fraction purities better than 0.97. Solid samples were purified by repeated crystallization or by fractional sublimation in vacuum. Liquid samples were purified by fractional distillation at reduced pressure in an inert atmosphere. Several compounds were used for measurements of solution enthalpies without purification (see Table S1). 2,4,6-Trinitrotoluene was synthesized from 2,4-dinitrotoluene according to a method from reference [9]. After synthesis it was recrystallized from ethanol and carbon tetrachloride.

Solvents used in this work were carefully purified before experiments using standard methodologies [10]. Benzene was washed with H_2SO_4, NaOH, water and distilled over CaH_2. Carbon tetrachloride and acetonitrile were fractionally distilled over P_2O_5. *N,N*-dimethylformamide was distillated over CaH_2 under reduced pressure.

The purity of samples was analyzed by gas chromatography (GC). An Agilent 7890 B gas chromatograph equipped with a flame ionization detector was used for this task. Water content was checked by Karl Fischer titration.

2.2. Solution calorimetry

Solution enthalpies for studied systems were measured at $T = 298.15 \pm 0.01$ K in concentration range from 0.5 to 241.0 mmol kg^{-1} using a TAM III solution calorimeter. Solid compounds were dissolved by breaking a glass ampule filled with 0.01–0.1 g of the studied sample in the glass cell with 100 ml of pure solvent. Liquid samples were injected by small portions (15–30 μl) using an electronically operated syringe equipped with a long gold cannula immersed in the solvent. The calorimeter was calibrated separately for these two types of input techniques, standardized by using the enthalpy associated with dissolving potassium chloride and propan-1-ol in pure water, respectively (Table S2). The average values of solution enthalpies of potassium chloride (17.41 ± 0.04 kJ mol^{-1}) and propan-1-ol (-10.16 ± 0.03 kJ mol^{-1}) in pure water are in excellent agreement with the recommended literature values (17.47 ± 0.07 kJ mol^{-1}) [11] (-10.16 ± 0.02 kJ mol^{-1}) [12]. The detailed information about the calorimetric procedure has been described elsewhere [13,14].

Solution enthalpies of the samples studied in this work at each concentration in carbon tetrachloride, benzene, acetonitrile and *N,N*-dimethylformamide are listed in Table S2.

3. Methodology

The enthalpy of solvation $\Delta_{soln}H^{A/S}$ is the enthalpy of isothermal transfer of solute A from the ideal gas state to an infinitely diluted solution in solvent S at 298.15 K and 0.1 MPa pressure. The solution enthalpy $\Delta_{soln}H^{A/S}$ is the enthalpy of transfer of solute A from its standard state (solid, liquid or vapor) to an infinitely diluted solution in solvent S at 298.15 K and 0.1 MPa pressure.

According to Eqs. (1) and (2) both the solution enthalpy at 298.15 K measured experimentally and the solvation enthalpy at 298.15 K are needed in order to determine vaporization and sublimation enthalpies for substance A. A value of $\Delta_{solv}H^{A/S}$ can be calculated from the linear correlations between solvation enthalpies and molar refractions (MR_A) [3–8]. Another way for calculation of solvation enthalpy is based on the use of multiparameter correlations. Best known of them were proposed by Acree and Abraham for different solvents [15–17]. Application of these correlations requires the knowledge of up to six independent parameters responsible for the specific type of intermolecular interactions present for the compound being studied.

Previously, various group contribution schemes were proposed for indirect determination of vaporization/sublimation enthalpies [1,7,18–21]. In present work we employed a group contribution approach for calculation of solvation enthalpies. In contrast to the enthalpy of phase transitions, the enthalpy of solvation of aromatic compounds in most cases does not depend on the position of substituents [7] and changes in the dipole moment [4,8] of molecules with the same composition. Therefore, the development of a group-contribution scheme for calculation of solvation enthalpies is a simpler task. Certainly, in some cases experimental values of solvation enthalpy can not be an additive function of group contributions, e.g., in systems where hydrogen bonds are formed between solute and solvent molecules, for example, a proton donor solute in a proton acceptor solvent. Consequently, alkanes and carbon tetrachloride should be the most suitable solvents for our method because they cannot form hydrogen bonds with either proton acceptors or with proton donors. Also, aprotic polar solvents can be used for studies of solutes which have only proton acceptor centers in order to simultaneously increase solubility and to avoid hydrogen bonding effects. However, even if a hydrogen bond between solute and solvent is formed in the system studied, its contribution still can be taken into account. This procedure will be discussed in detail in our further work.

The solvation enthalpy of aromatic or heteroaromatic compound (ArX_n) in any solvent (S) according to the group-contribution method proposed in this work is calculated as a sum of the solvation enthalpy of the reference unit (aromatic hydrocarbon;

heteroaromatic compound without substituent, for example, pyridine) and contributions due to the substitution of the hydrogen atoms in the reference unit by any other groups (X). This procedure can be described by Eq. (3).

$$\Delta_{solv}H^{ArX_n/S} = \Delta_{solv}H^{ArH/S} + n \cdot \Delta_{solv}H^{X\rightarrow H/S} \quad (3)$$

where, $\Delta_{solv}H^{ArX_n/S}$ is the solvation enthalpy of the aromatic or heteroaromatic compound in solvent S; $\Delta_{solv}H^{ArH/S}$ is the solvation enthalpy of parent molecule in the same solvent S; $\Delta_{solv}H^{X\rightarrow H/S}$ is the contribution to the solvation enthalpy related to the substitution of a hydrogen atom in the reference unit by the substituent X; n is the number of substituents.

Solvation enthalpies of aromatic hydrocarbons and heteroaromatic compounds without substituents ($\Delta_{solv}H^{ArH/S}$) required for using of Eq. (3) can be determined from the experimental data on solution enthalpies in the same solvent ($\Delta_{soln}H^{ArH/S}$) and vaporization/sublimation enthalpies ($\Delta^{g}_{cr,l}H^{ArH}$) according to Eq. (4). For many aromatic hydrocarbons enthalpies of vaporization/sublimation were determined many times and recommended values are available in the literature [22].

$$\Delta_{solv}H^{ArH/S} = \Delta_{soln}H^{ArH/S} - \Delta^{g}_{cr,l}H^{ArH} \quad (4)$$

Group contributions due to the substitution of hydrogen atom by other groups were calculated as the difference between enthalpy of solvation of monosubstituted benzene and benzene (Eq. (5)).

$$\Delta_{solv}H^{X\rightarrow H/S} = \Delta_{solv}H^{C_6H_5X/S} - \Delta_{solv}H^{C_6H_6/S} \quad (5)$$

Values of $\Delta_{solv}H^{X\rightarrow H/S}$ obtained this way for 16 substituents in four solvents are presented in Table 1. It is evident from Table 1 that values of $\Delta_{solv}H^{X\rightarrow H/S}$ for proton donor groups (OH, NH_2 and $CONH_2$) are changed dramatically depending on the solvent selected. The reason is the possibility of hydrogen bond formation between these groups and some of the chosen solvents. Values of $\Delta_{solv}H^{X\rightarrow H/S}$ for other groups were less dependent on the solvent. Contribution to the solvation enthalpy due to substitution of hydrogen atom by F is close to zero. The largest value of $\Delta_{solv}H^{X\rightarrow H/S}$ was obtained for $CONH_2$ group. The list of group contributions obtained in this paper is not final and will be expanded in our future work. For two systems studied in this work (toluene in benzene and benzonitrile in benzene) literature values on solution enthalpies were available. Comparison of our and literature data has shown, that solution enthalpies of benzonitrile in benzene measured in this work (0.54 ± 0.08 kJ mol^{-1}) and obtained in [24] (0.5 kJ mol^{-1}) are practically indistinguishable. For toluene in benzene small difference between our data (0.28 ± 0.01 kJ mol^{-1}) and measured in [23] (0.5 ± 0.2 kJ mol^{-1}) is observed. In work [23] authors did not analyze purity of studied samples and water content, also they did not identify the method of purification of solutes and solvents. In our work we have distillated toluene as well as benzene and have analyzed their purity. Therefore, we consider that solution enthalpy measured in our work is more correct and we used it for further calculations.

In this work, we have taken several aromatic hydrocarbons (benzene, naphthalene, biphenyl, anthracene and pyrene) and pyridine as reference units for calculation solvation enthalpies of their derivatives. We have determined their enthalpies of solvation in four solvents (carbon tetrachloride, benzene, *N,N*-dimethylformamide and acetonitrile) using Eq. (4). Table 2 contains obtained results for $\Delta_{solv}H^{ArH/S}$. Enthalpies of solution of aromatic hydrocarbons and pyridine used for calculations are presented in Table S2. The details of the calculations are fully described in Supplementary material.

On the basis of Eqs. (1) and (2) and a group contribution scheme for calculation of solvation enthalpies (Eqs. (3)–(5)), we developed a method for determination of vaporization/sublimation enthalpies which is based on Eq. (6) for liquid compounds and Eq. (7) for solids at the standard state:

$$\Delta^{g}_{l}H^{Ar(X)_n}_{m} = \Delta_{soln}H^{Ar(X)_n/S} - \Delta_{solv}H^{ArH/S} - n \cdot \Delta_{solv}H^{X\rightarrow H/S} \quad (6)$$

$$\Delta^{g}_{cr}H^{Ar(X)_n}_{m} = \Delta_{soln}H^{Ar(X)_n/S} - \Delta_{solv}H^{ArH/S} - n \cdot \Delta_{solv}H^{X\rightarrow H/S} \quad (7)$$

Eqs. (6) and (7) give opportunity to access phase transition enthalpies of aromatic and heteroaromatic compounds directly at 298.15 K without any temperature adjustment. The only one parameter needed to be measured in order to apply this method is the enthalpy of solution, the remaining values in Eqs. (6) and (7) can be taken from Tables 1 and 2. In addition, if the studied compound is poorly soluble in carbon tetrachloride or benzene, then acetonitrile or *N,N*-dimethylformamide can be used instead or vice versa. Vaporization/sublimation enthalpy obtained by Eqs. (6) and (7) does not depend on the choice of solvent. This fact significantly extends the application of the solution calorimetry approach.

4. Results and discussion

In this work we have applied Eqs. (6) and (7) for determination of vaporization/sublimation enthalpies of different aromatic and heteroaromatic compounds, which include derivatives of benzene, pyridine, naphthalene, biphenyl, anthracene and pyrene. Enthalpies of solution at infinite dilution for 43 solute-solvent systems were measured at 298.15 K. Part of these values together with available literature data are presented in Table 3 for carbon tetrachloride as a solvent, in Table 4 for benzene as a solvent, in Table 5 for acetonitrile as a solvent and in Table 6 for *N,N*-dimethylformamide as a solvent. These solvents were chosen because they have different solvating ability (from non-polar to highly polar). Dissolution processes for all solutes studied are endothermic except dissolution of 1-bromo-3-chlorobenzene, 1,3-dibromobenzene and 3-methylaniline in *N,N*-dimethylformamide. The latter system has the most negative solution enthalpy due to formation of solute–solvent hydrogen bonds. Solid compounds have always larger values of $\Delta_{soln}H^{A_i/S}$ due to breaking of the crystal lattice upon dissolution. Solvation enthalpies of compounds studied in four solvents were calculated by an additive scheme (Eq. (3)) using the solvation enthalpies of the reference units (Table 2) and the group contribution values (Table 1). These values are also presented in Tables 3–6. Solvation enthalpies of 1-naphthol and 2-naphthol in acetonitrile and *N,N*-dimethylformamide were calculated using solvation enthalpy of naphthalene and OH-group contribution, respectively. This is possible, because enthalpies of hydrogen bonding between respective naphthols and acetonitrile or *N,N*-dimethylformamide are equal to values obtained for phenol (the model compound for determination of OH-group contribution) [25]. Vaporization and sublimation enthalpies reported in the fourth column of Tables 3–6 were obtained from measured solution enthalpies and calculated solvation enthalpies using Eqs. (6) and (7).

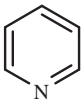
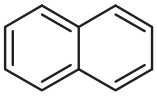
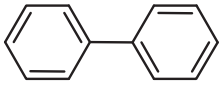
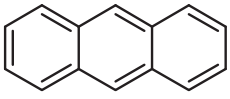
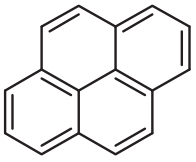
As a matter of the fact, results obtained for $\Delta^{g}_{cr,l}H^{Ar(X)_n}$ confirm that the choice of solvent does not affect the enthalpy values. Enthalpies of sublimation of 4-nitrotoluene (I), 1-chloro-2-nitrobenzene (II) and 1-chloro-3-nitrobenzene (III) evaluated from the solution and solvation enthalpies of these species in benzene (Table 4) ($\Delta^{g}_{cr}H^{I} = 74.9$ kJ mol^{-1}; $\Delta^{g}_{cr}H^{II} = 79.2$ kJ mol^{-1}; $\Delta^{g}_{cr}H^{III} = 82.2$ kJ mol^{-1}) are indistinguishable within the experimental uncertainties from the enthalpies of sublimation of these compounds obtained from the solution and solvation enthalpies in acetonitrile (Table 4) ($\Delta^{g}_{cr}H^{I} = 75.4$ kJ mol^{-1}; $\Delta^{g}_{cr}H^{II} = 80.1$ kJ mol^{-1}; $\Delta^{g}_{cr}H^{III} = 83.1$ kJ mol^{-1}). It should be noted that values obtained for $\Delta^{g}_{cr,l}H^{Ar(X)_n}$ of isomers are significantly different due to the different physical state (liquid or solid) of the molecules due to different energy costs on breaking of the

Table 1
Group contributions to the enthalpy of solvation in carbon tetrachloride, benzene, acetonitrile and *N*,*N*-dimethylformamide (DMF) calculated by Eq. (5) (all values at 298.15 K).

1	$-\Delta_{solv}H^{X\rightarrow H/CCl_4}$ (kJ mol^{-1}) 2	$-\Delta_{solv}H^{X\rightarrow H/C_6Cl_6}$ (kJ mol^{-1}) 3	$-\Delta_{solv}H^{X\rightarrow H/CH_3CN}$ (kJ mol^{-1}) 4	$-\Delta_{solv}H^{X\rightarrow H/DMF}$ (kJ mol^{-1}) 5
CH_3	4.6	3.5	3.3	3.3
t-C_4H_9	13.7	12.0	10.6	10.2
F	−0.8	−0.4	0.7	1.3
Cl	6.2	6.1	6.0	7.4
Br	8.7	8.7	8.4	9.9
I[a]	14.5	14.7	13.2	17.3
NO_2	16.0	17.9	21.0	21.2
CHO	13.7	15.5	17.5	17.9
NH_2	13.0	15.8	23.6	32.4
CN	12.7	15.8	17.5	18.5
CH_3O	10.9	11.6	12.4	11.8
$COCH_3$	18.4	19.6	22.0	21.7
$N(CH_3)_2$	18.7	18.2	18.3	18.4
OH	8.3	14.2	27.2	38.7
$CONH_2$	–	40.8	47.3	59.8
$COOCH_3$	19.1	20.4	21.1	20.7

[a] Enthalpy of solvation of iodobenzene in studied solvents required for determination of group contributions of I-group was obtained by method proposed in [4] from molar refraction values.

Table 2
Solvation enthalpies of aromatic hydrocarbons and pyridine in carbon tetrachloride, benzene, acetonitrile and *N*,*N*-dimethylformamide (DMF) calculated from vaporization or sublimation enthalpies and solution enthalpies (all values at 298.15 K) by Eq. (4).

1	$-\Delta_{solv}H^{ArH/CCl_4}$ (kJ mol^{-1}) 2	$-\Delta_{solv}H^{ArH/C_6H_6}$ (kJ mol^{-1}) 3	$-\Delta_{solv}H^{ArH/CH_3CN}$ (kJ mol^{-1}) 4	$-\Delta_{solv}H^{ArH/DMF}$ (kJ mol^{-1}) 5
	34.2	34.8	32.2	34.6
	38.9	40.2	38.5	40.6
	53.9	54.9	51.2	56.3
	63.6	63.9	60.7	66.6
	77.4	77.2	74.0	79.6
	–	87.6	82.3	–

crystal lattice upon sublimation of solid compounds. At the same time solvation enthalpies of isomers in each solvent are equal.

In order to test the reliability of the method proposed in this work we decided to compare our results with data on vaporization/sublimation enthalpies of compounds determined by conventional methods available in the literature [7,27,29,30,32,34,36,38,39,41–44,47,48,50,52,54–80,82–88].
Results of comparison show (Tables 3–6) that for 34 systems, the difference between solution calorimetry results and the values obtained by conventional methods is less than 1 kJ mol^{-1}, for 42 compounds this difference lies in the range of 1–3 kJ mol^{-1} and only for 5 compounds it is higher than 3 kJ mol^{-1}. The observed differences could arise because of the experimental uncertainties in measurements of solution enthalpies, experimental uncertainties in measurements of vaporization/sublimation enthalpies and uncertainties in their adjustment to the reference temperature 298.15 K. Of course, uncertainties in the additive scheme for calculation of solvation enthalpies proposed in this work also can affect the coincidence of our and literature results. In total 78 aromatic and heteroaromatic compounds studied here cover the range of vaporization/sublimation enthalpies from 34.5 kJ mol^{-1} (1,2-difluorobenzene) to 127.1 kJ mol^{-1} (1-nitropyrene). The average deviation between vaporization/sublimation enthalpies obtained in the present work by solution calorimetry and literature data determined by different conventional methods is less than 2%. Excellent agreement of data on the vaporization/sublimation enthalpies for a wide range of values (about 100 kJ mol^{-1}) and for different classes of aromatic compounds fully confirms the reliability of the proposed approach and allows to use it successfully for other aromatic and heteroaromatic compounds. Unlike conventional methods, solution calorimetry approach requires only the measurement of solution enthalpy of the compound in

Table 3
Enthalpies of solution and enthalpies of solvation of aromatic compounds in carbon tetrachloride and their vaporization/sublimation enthalpies (all values at 298.15 K).

N	Compound $(Ar(X)_n)$	$\Delta_{soln}H^{ArX_n/CCl_4}$ [a] (kJ mol^{-1})	$-\Delta_{solv}H^{ArX_n/CCl_4}$ [c] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (this work)[d] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (lit.)[e] (kJ mol^{-1})	Δ[f] (kJ mol^{-1})	RE[g] (%)
1	1,4-Difluorobenzene (l)	1.9 [26]	32.6	34.5	36.0 ± 0.2 [27]	1.5	4.2
2	2-Chlorophenol (l)	6.0 [28]	48.7	54.7	52.3 ± 0.2 [29]	2.4	4.6
3	2-Bromophenol (l)	5.0 [28]	51.2	56.2	55.5 ± 1.3 [30]	0.7	1.3
4	3-Fluorophenol (l)	15.9 [31]	41.7	57.6	60.1 ± 0.9 [32]	2.5	4.2
5	2-Methoxyphenol (l)	8.6 [33]	53.4	62.0	61.4 ± 0.3 [34]	0.6	1.0
6	3-Methyphenol (l)	15.6 [35]	47.1	62.7	61.7 ± 1.0 [36]	1.0	1.6
7	3-Methoxyphenol (l)	16.0 [28]	53.4	69.4	74.8 ± 0.2[34]	4.1	7.2
8	Pentafluorophenol (cr)	32.0 [37]	38.5	70.5	67.4 ± 1.7 [38]	3.1	4.6
9	4-Fluorophenol (cr)	29.3 [26]	41.7	71.0	73.9 ± 1.4 [32]	2.9	3.9
10	4-Chlorophenol (cr)	28.6[b]	48.7	77.3	77.1 ± 0.2[29]	0.2	0.3
11	3-Chlorophenol (cr)	29.0 [28]	48.7	77.7	76.9 ± 0.3[29]	0.8	1.0
12	3-Bromophenol (cr)	27.0 [28]	51.2	78.2	76.3 [39]	1.9	2.5
13	4-Bromophenol (cr)	28.0 [28]	51.2	79.2	83.1 ± 0.1 [30]	3.9	4.7
14	Hexamethylbenzene (cr)	20.8 [40]	61.8	82.6	81.4 ± 0.1 [41]	1.2	1.5
15	2,4,6-Trimethylphenol (cr)	26.6[b]	56.3	82.9	82.8 ± 0.3 [42]	0.1	0.1
16	4-*tert*-Butylphenol (cr)	27.2[b]	56.2	83.4	85.9 ± 0.5 [43]	2.5	2.9
17	1,2,4,5-Tetrachlorobenzene (cr)	25.1 [4]	59.0	84.1	83.2 ± 0.3 [44]	0.9	1.1
18	2,6-Di-*tert*-butylphenol (cr)	16.1 [45]	69.9	86.0	84.6 ± 0.5 [42]	1.4	1.6
19	2,4-Di-*tert*-butylphenol (cr)	16.7[b]	69.9	86.6	86.7 ± 0.3 [43]	0.1	0.1
20	4-Methoxyphenol (cr)	37.0 [28]	53.4	90.4	89.8 ± 0.3[34]	0.6	0.7
21	Hexachlorobenzene (cr)	24.3 [4]	71.4	95.7	96.8 ± 0.5 [29]	1.1	1.1

[a] Enthalpy of solution of aromatic compounds in carbon tetrachloride at 298.15 K.
[b] Enthalpy of solution measured in this work.
[c] Enthalpy of solvation of aromatic compounds in carbon tetrachloride at 298.15 K.
[d] Vaporization/sublimation enthalpy of aromatic compounds determined by Eqs. (6) and (7) at 298.15 K.
[e] Literature values of vaporization/sublimation enthalpy of aromatic compounds at 298.15 K.
[f] Absolute difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.
[g] Relative difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.

Table 4
Enthalpies of solution and enthalpies of solvation of aromatic compounds in benzene and their vaporization/sublimation enthalpies (all values at 298.15 K).

N	Compound $(Ar(X)_n)$	$\Delta_{soln}H^{ArX_n/C_6H_6}$ [a] (kJ mol^{-1})	$-\Delta_{solv}H^{ArX_n/C_6H_6}$ [c] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (this work)[d] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (lit.)[e] (kJ mol^{-1})	Δ[f] (kJ mol^{-1})	RE[g] (%)
1	Pentafluorobenzene (l)	1.0 [46]	32.8	33.8	36.2 ± 0.2 [38]	2.4	6.6
2	1,2,4,5-Tetrafluorobenzene (l)	1.5 [46]	33.2	34.7	37.1 ± 1.0 [47]	2.4	6.5
3	1,4-Dimethylbenzene (l)	1.05 [23]	41.8	42.9	42.3 ± 0.1 [48]	0.6	1.4
4	2-Methylpyridine (l)	0.1 [49]	43.7	43.8	42.5 ± 0.3 [50]	1.3	3.1
5	4-Fluoroanisole (l)	0 [26]	46.0	46.0	48.7 ± 1.1 [51]	2.7	5.5
6	3-Chloropyridine (l)	1.02 [49]	46.3	47.3	47.9 ± 1.1 [52]	0.6	1.3
7	2,6-Dimethylpyridine (l)	0.4 [49]	47.2	47.6	45.4 ± 0.3 [50]	2.2	4.8
8	2,4-Dimethylpyridine (l)	0.5 [49]	47.2	47.7	47.5 ± 0.3 [50	0.2	0.4
9	1,3,5-Trimethylbenzene (l)	2.6 [53]	45.3	47.9	47.5 ± 0.2 [54]	0.4	0.8
10	2-Chloroaniline (l)	2.0[b]	56.7	58.7	57.1 ± 0.5 [55]	1.6	2.8
11	1-Chloronaphthalene (l)	1.0 [4]	61.0	62.0	62.0 ± 0.4 [56]	0.0	0.0
12	1-Bromonaphthalene (l)	1.24 [7]	63.6	64.8	63.7 ± 0.9 [7]	1.1	1.7
13	1-Iodonaphthalene (l)	1.7 [7]	68.2	71.3	69.9 ± 0.6 [56]	1.4	2.0
14	3-Cyanopyridine (cr)	18.0 [49]	56.0	74.0	72.1 ± 1.8 [57]	1.9	2.6
15	4-Cyanopyridine (cr)	18.2 [49]	56.0	74.2	73.2 ± 0.6 [57]	1.0	1.4
16	4-Nitrotoluene (cr)	18.7[b]	56.2	74.9	74.8 ± 1.0 [58]	0.1	0.1
17	4-Bromoaniline (cr)	19.6[b]	59.3	78.9	79.4 ± 1.7 [59]	0.5	0.6
18	1-Chloro-2-Nitrobenzene (cr)	20.4[b]	58.8	79.2	80.8 ± 0.3 [55]	1.6	2.0
19	1-Chloro-3-Nitrobenzene (cr)	23.4[b]	58.8	82.2	81.3 ± 0.3 [55]	0.9	1.1
20	4-Iodoaniline (cr)	21.2[b]	63.9	86.5	84.8 ± 1.4 [60]	1.7	2.0
21	1-Aminonaphthalene (cr)	19.1[b]	70.7	89.8	88.1 ± 0.4 [61]	1.7	1.9
22	2-Nitroaniline (cr)	23.1[b]	68.5	91.6	90.0 ± 3.0 [62]	1.6	1.8
23	1,4-Dibromonaphthalene (cr)	20.6 [7]	72.3	92.9	91.3 ± 1.4 [63]	1.6	1.7
24	o-Phenylenediamine (cr)	26.6[b]	66.4	93.0	89.8 ± 0.4 [64]	3.2	3.6
25	p-Phenylenediamine (cr)	28.5[b]	66.4	94.9	96.8 ± 0.4 [64]	1.9	2.0
26	3-Nitroaniline (cr)	26.5[b]	68.5	95.0	97.0 ± 1.0 [65]	2.0	2.1
27	9,10-Dibromoanthracene (cr)	24.8 [7]	94.6	119.4	117.5 ± 3.0 [63]	1.9	1.6
28	1-Nitropyrene (cr)	21.6[b]	105.5	127.1	125.2 ± 3.8 [66]	1.9	1.5

[a] Enthalpy of solution of aromatic compounds in benzene at 298.15 K.
[b] Enthalpy of solution measured in this work.
[c] Enthalpy of solvation of aromatic compounds in benzene at 298.15 K.
[d] Vaporization/sublimation enthalpy of aromatic compounds determined by Eqs. (6) and (7) at 298.15 K.
[e] Literature values of vaporization/sublimation enthalpy of aromatic compounds at 298.15 K.
[f] Absolute difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.
[g] Relative difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.

Table 5
Enthalpies of solution and enthalpies of solvation of aromatic compounds in acetonitrile and their vaporization/sublimation enthalpies (all values at 298.15 K).

N	Compound $(Ar(X)_n)$	$\Delta_{soln}H^{ArX_n/CH_3CN}$ [a] (kJ mol^{-1})	$-\Delta_{solv}H^{ArX_n/CH_3CN}$ [c] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (this work) [d] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (lit.) [e] (kJ mol^{-1})	Δ [f] (kJ mol^{-1})	RE [g] (%)
1	1,2-Dichlorobenzene (l)	3.9 [4]	44.2	48.1	49.9 [67]	1.8	3.6
2	2-Nitrotoluene (l)	3.0 [b]	56.5	59.5	59.1 ± 0.3 [68]	0.4	0.7
3	1,4-Dichlorobenzene (cr)	21.2 [4]	44.2	65.4	64.8 ± 0.2 [69]	0.6	0.9
4	4-Nitrotoluene (cr)	18.9 [b]	56.5	75.4	74.8 ± 1.0 [58]	0.6	0.8
5	Dimethyl phthalate (l)	1.5 [b]	74.4	75.9	77.0 ± 1.2 [70]	1.1	1.4
6	1-Chloro-4-nitrobenzene (cr)	17.2 [5]	59.2	76.4	74.7 ± 0.2 [55]	1.7	2.3
7	1-Chloro-2-nitrobenzene (cr)	20.9 [b]	59.2	80.1	80.8 ± 0.3 [55]	0.7	0.9
8	1-Chloro-3-nitrobenzene (cr)	23.9 [b]	59.2	83.1	81.3 ± 0.3 [55]	1.8	2.2
9	1-Bromo-4-nitrobenzene (cr)	24.3 [b]	61.6	85.9	86.6 ± 0.6 [71]	0.7	0.8
10	1,3-Dinitrobenzene (cr)	15.5 [4]	74.2	89.7	87.0 ± 4.0 [72]	2.7	3.1
11	1,4-Dicyanobenzene (cr)	22.7 [b]	67.2	89.9	89.7 ± 1.8 [73]	0.2	0.2
12	1-Naphthol (cr)	13.6 [5]	78.4	92.0	91.2 ± 0.4 [74]	0.8	0.9
13	1-Nitronaphthalene (cr)	22.3 [4]	72.2	94.5	95.1 ± 0.4 [75]	0.6	0.6
14	1,2-Dinitrobenzene (cr)	21.3 [4]	74.2	95.5	95.5 ± 0.9 [76]	0.0	0.0
15	1,4-Dinitrobenzene (cr)	21.3 [4]	74.2	95.5	94.3 ± 0.7 [76]	1.2	1.3
16	2,4-Dinitrotoluene (cr)	21.4 [b]	77.5	98.9	99.4 ± 2.5 [77]	0.5	0.5
17	Dimethyl terephthalate (cr)	30.0 [b]	74.4	104.4	104.6 ± 0.3 [78]	0.2	0.2
18	9-Nitroanthracene (cr)	22.4 [b]	95.0	117.4	115.4 ± 0.6 [75]	2.0	1.7
19	2,4,6-Trinitrotoluene (cr)	19.2 [b]	98.5	117.7	118.4 ± 4.2 [79]	0.7	0.6
20	3-Methoxybenzamide (cr)	28.2 [b]	91.9	120.1	119.8 ± 0.4 [80]	0.3	0.3

[a] Enthalpy of solution of aromatic compounds in acetonitrile at 298.15 K.
[b] Enthalpy of solution measured in this work.
[c] Enthalpy of solvation of aromatic compounds in acetonitrile at 298.15 K.
[d] Vaporization/sublimation enthalpy of aromatic compounds determined by Eqs. (6) and (7) at 298.15 K.
[e] Literature values of vaporization/sublimation enthalpy of aromatic compounds at 298.15 K.
[f] Absolute difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.
[g] Relative difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.

Table 6
Enthalpies of solution and enthalpies of solvation of aromatic compounds in *N*,*N*-dimethylformamide (DMF) and their vaporization/sublimation enthalpies (all values at 298.15 K).

N	Compound $(Ar(X)_n)$	$\Delta_{soln}H^{ArX_n/DMF}$ [a] (kJ mol^{-1})	$-\Delta_{solv}H^{ArX_n/DMF}$ [b] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (this work) [c] (kJ mol^{-1})	$\Delta^g_{cr,l}H^{ArX_n}$ (lit.) [d] (kJ mol^{-1})	Δ [e] (kJ mol^{-1})	RE [f] (%)
1	1-Bromo-3-chlorobenzene (l)	−0.6 [81]	51.9	51.3	51.3 ± 0.4 [82]	0.0	0.0
2	1,3-Dibromobenzene (l)	−0.4 [81]	54.4	54.0	54.9 ± 0.6 [7]	0.9	1.6
3	3-Methylaniline (l)	−11.2 [81]	70.3	59.1	58.3 ± 0.4 [83]	0.8	1.4
4	1,4-Di-*tert*-butylbenzene (cr)	25.9 [81]	55.0	80.9	82.8 ± 0.4 [84]	1.9	2.3
5	2,4,6-Trimethylnitrobenzene (cr)	16.7 [81]	65.7	82.4	78.6 ± 1.0 [85]	3.8	4.8
6	1-Bromo-3-nitrobenzene (cr)	19.2 [81]	65.7	84.9	86.8 ± 0.5 [71]	1.9	2.2
7	1-Iodo-3-nitrobenzene (cr)	15.1 [81]	73.1	88.2	88.8 ± 0.5 [86]	0.6	0.7
8	1-Iodo-4-nitrobenzene (cr)	19.2 [81]	73.1	92.3	94.6 ± 0.6 [86]	2.3	2.4
9	1-Dimethylamino-3-nitrobenzene (cr)	19.7 [81]	74.2	93.9	92.7 ± 0.3 [87]	1.2	1.3
10	2-Naphthol (cr)	0.0 [81]	95.0	95.0	94.2 ± 0.5 [74]	0.8	0.8
11	4-Nitroacetophenone (cr)	17.6 [81]	77.5	95.1	96.5 ± 0.5 [88]	1.4	1.5
12	3-Nitroacetophenone (cr)	18.8 [81]	77.5	96.3	98.6 ± 0.6 [88]	2.3	2.3

[a] Enthalpy of solution of aromatic compounds in *N*,*N*-dimethylformamide at 298.15 K.
[b] Enthalpy of solvation of aromatic compounds in *N*,*N*-dimethylformamide at 298.15 K.
[c] Vaporization/sublimation enthalpy of aromatic compounds determined by Eqs. (6) and (7) at 298.15 K.
[d] Literature values of vaporization/sublimation enthalpy of aromatic compounds at 298.15 K.
[e] Absolute difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.
[f] Relative difference between vaporization/sublimation enthalpies obtained in this work and taken from literature.

one of the chosen solvents at a temperature 298.15 K directly. Consequently, the necessity of temperature adjustment is absent in this case.

A number of group-contribution methods for prediction of vaporization/sublimation enthalpies were proposed up to the present date [1,7,18–21]. We would like to comment on the key differences between these methods and our approach.

First, the physical state of the compound does not matter for our group contribution scheme. It could be solid or liquid, nevertheless the group-contribution values for calculation of vaporization/sublimation enthalpies by Eqs. (6) and (7) will be the same, respectively. In case of methods proposed in literature [1,18–21], contributions for the same group will be different for determination of vaporization or sublimation enthalpies due to additional term for breaking the crystal lattice of solid compounds. Second, our approach does not require contributions due to the position of substitution in aromatic or heteroaromatic ring. The enthalpies of solvation of *ortho*-, *meta*- and *para*-isomers of any compound studied in each solvent are equal (see Tables 3–6). Some exceptions are possible only for molecules with intramolecular hydrogen bonds. Vaporization/sublimation enthalpies of aromatic compounds in a majority of cases are different for *ortho*-, *meta*- and *para*-isomers (see Tables 3–6). Therefore, for application of existing group-contribution schemes [1,18–21] for the prediction of $\Delta^g_{cr,l}H^{Ar(X)_n}$ values, additional contributions need to be taken into account both for systems with and without intramolecular hydrogen bonds. Third, there is one fundamental unclear assumption in case of existing group-contribution methods for prediction

of $\Delta^{g}_{cr,l}H^{Ar(X)_n}$ values. The enthalpy of solution of liquid compound A in itself is equal to zero. Consequently, according to Eq. (1) the vaporization enthalpy of compound A equals to the negative solvation enthalpy of A in itself. In accordance to the group-contribution approach, the enthalpy of vaporization is calculated on the basis of the vaporization enthalpies of model compounds. It follows that the solvation of groups could be different in the compound studied and model compounds used to determine increments. For example, if the compound of interest is an aromatic derivative ArXY, the increments for groups X and Y would be used. However, it is possible that the solvation of X and Y in ArXY would be different from the solvation of X and Y in their respective model compounds ArX and ArY, because the compound of interest and compounds used to calculate group contribution represent different solvation media. The differences in solvation enthalpy control the discrepancies between values calculated using an additive scheme and measured values of the vaporization enthalpy. In case of sublimation another contribution appears namely the fusion enthalpy which can hardly be considered additive in general. The latter circumstance makes attempts to calculate sublimation enthalpies using an additive scheme even more difficult. In our case calculation of solvation enthalpy additively implies solvation of groups as well as the complete molecule in the same single solvent. In the absence of H-bonding between solvent and solute the additivity in solvation enthalpies is well realized. However, solution enthalpy must be measured in the same solvent to calculate the vaporization/sublimation enthalpy. In fact, our method for vaporization/sublimation enthalpy determination is a hybrid of group-contribution and experimental approaches.

5. Conclusion

In this work we have proposed a new method for the determination of vaporization/sublimation enthalpy of aromatic and heteroaromatic compounds at 298.15 K. The method is based on experimental measurement of solution enthalpy and calculation of solvation enthalpy in a selected solvent. The latter values are calculated using an additive scheme from the solvation enthalpy of parent compound (aromatic hydrocarbons and heteroaromatic units) and group contributions of substituents. Our method can be applied also for compounds that contain aromatic or heteroaromatic fragments as a substituent. Results of vaporization/sublimation enthalpies obtained by solution calorimetry approach do not depend on the choice of solvent and they are in good agreement with available literature data for all 78 compounds studied.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.tca.2015.09.022.

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