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Research paper

Sublimation enthalpy of 1-aminoadamantane: Comparison of theory and experiment

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HIGHLIGHTS

- Sublimation enthalpies are predicted using electrostatic potential model.
- Model provides a good agreement with experiment except for 1-aminoadamantane.
- Discrepancy may be due to not totally crystalline phase of 1-aminoadamantane.
- Plastic crystals should be rejected in developing the estimation methods.

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ABSTRACT

The sublimation enthalpy of 1-aminoadamantane was estimated using the molecular electrostatic potential (MEP) model. An equation has been proposed that describes the relationship between the sublimation enthalpy and computed crystal density, molecular surface area plus four quantities obtained from the surface electrostatic potential. The coefficients in this equation were determined from least-squares fitting to reliable values of sublimation enthalpy of 23 adamantanes. The sublimation enthalpies estimated by MEP model agree within 4 kJ·mol^{-1} for all compounds, except for 1-aminoadamantane. The reason for a large difference between experimental and estimated sublimation enthalpy of 1-aminoadamantane is discussed.

1. Introduction

Aminoadamantanes, amantadine (1-aminoadamantane) and rimantadine (α-methyl-1-adamantanemethylamine), were among the first drugs that successfully made it to the pharmaceutical market, and they are still being used to date [1]. Experimental thermochemical data for 1-aminoadamantane were not reported for a long time, probably because of its high reactivity, and they have been published only in 2008 by Bazyleva et al. [2]. From the temperature dependence of the saturated vapor pressure, the sublimation enthalpy at 298.15 K ($\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{\circ}$) was determined to be 61.7 ± 0.6 kJ·mol^{-1}. Later, Gobble et al. [3] paid attention that for a crystalline solid melting at $T = 480$ K, this value appeared surprisingly small especially since a simple group additivity equation predicted a vaporization enthalpy of approximately 60 kJ·mol^{-1}. However, the experimental sublimation enthalpy [2] was supported by Gobble et al. [3] from their own measurements: the vaporization enthalpy (59.9 ± 2.5 kJ·mol^{-1}) combined with a possible fusion enthalpy of up to 1.5 kJ·mol^{-1} results in a sublimation enthalpy of ~61.4 ± 3.5 kJ·mol^{-1}. It should be noted that efforts to obtain a crystal structure of 1-aminoadamantane at room temperature were unsuccessful, and the enthalpy of fusion was measured for a partially crystalline phase.

In this work, we decided to try to estimate the sublimation enthalpy of 1-aminoadamantane following ideas introduced by Politzer and coworkers [4–7], who have shown that a number of physical properties, including enthalpies of sublimation and vaporization, may often be expressed in terms of molecular descriptors defined from the molecular electrostatic potential (MEP). This model has found application for prediction of sublimation enthalpies of energetic compounds [8,9], and the most accurate results were obtained when the approach was applied to structurally similar compounds [10,11]. It is obviously, that the accuracy of the predictions will depend on the accuracy of the experimental data used for model calibration. In our recent work [12], we have analyzed the accuracy of available experimental data on gas-phase enthalpies of formation of adamantanes using isodesmic reactions network, and thus we can select the reliable $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{\circ}$ values whose accuracy was confirmed by indirect theoretical calculations.

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2. Computational details

Politzer et al. [4,6] have shown that a variety of physical properties can be expressed quantitatively in terms of overall molecular surface area (A_S) plus quantities obtained from the surface electrostatic potential:

$$\text{Property} = f(A_S, V_{S,\min}, V_{S,\max}, \bar{V}_S^+, \bar{V}_S^-, \Pi, \sigma_+^2, \sigma_-^2, \sigma_{\mathrm{tot}}^2, \nu, A_S^+, A_S^-) \qquad (1)$$

where $V_{S,\min}$ and $V_{S,\max}$ are the most negative and most positive values of the molecular surface electrostatic potential, $\bar{V}_S^+$ and $\bar{V}_S^-$ are the average positive and negative potentials over the entire surface, Π is the average deviation of the electrostatic potential on the molecular surface (a measure of local polarity), σ_{tot}^2 indicates the variability of the potential on the molecular surface and it equals to the sum of the variances of the positive and negative regions of surface potential, σ_+^2 and σ_-^2, ν is the degree of the balance between positive and negative regions, and A_S^+ and A_S^- are the positive and negative surface areas. The expressions proposed for different properties normally involve, in various combinations, only three or four of the quantities on the right side of Eq. (1). Thus, the equation for sublimation enthalpy [5] involves surface area and two surface electrostatic potential quantities:

$$\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{\circ} = a(A_S)^2 + b\sqrt{\sigma_{\mathrm{tot}}^2\nu} + c \qquad (2)$$

The parameters a, b, and c in Eq. (2) were determined in Ref. [5] from least squares fitting to reliable values of the enthalpies of sublimation of 34 organic compounds of various types. All calculations were carried out at the ab initio HF/STO-5G(d)//HF/STO-3G(d) level. Later Eq. (2) was applied to 66 experimental enthalpies of sublimation using the higher level computational method B3PW91/6-31G(d,p) [7]. The most widely used coefficients a, b, and c in Eq. (2) were obtained by Byrd and Rice [8] using 23 energetic compounds in the parametrization of this equation and the B3LYP/6-311++G(2df,2p)//B3LYP/6-31G(d) method to determine the densities for generating the MEPs. Some authors proposed the equations that are different from Eq. (2) [13,14,11]. In particular, Mathieu and Bougrat [13] suggested using the linear dependence of sublimation enthalpy on A_S rather than the quadratic dependence.

In this work, the DFT/B3LYP/6-311++G(3df,2p) method was used to optimize geometries and determine the densities for generating the electrostatic potentials. Along with Eq. (2), we considered other equations with different number and various combinations of descriptors given in Eq. (1). The best results are obtained for equation which, compared to Eq. (2), has additional molecular descriptors, ρ (crystal density), $\bar{V}_S$ (the average value of the potential on the surface), Π (the measure of local polarity), and shows a linear sublimation enthalpy dependence on A_S and $\sigma_{\mathrm{tot}}^2\nu$:

$$\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{\circ} = a\rho + bA_S + c\bar{V}_S + d(\sigma_{\mathrm{tot}}^2\nu) + e\Pi + f \qquad (3)$$

This equation is characterized by better agreement between the calculated and experimental enthalpies of sublimation. For a set of 23 adamantanes, the $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{\circ}$ values predicted using the Eq. (3) produce a root-mean-square deviation (RMSD) of 3.7 kJ·mol^{-1}, compared to 6.3 kJ·mol^{-1} for the same molecules using the Eq. (2).

All descriptors in Eq. (3) were calculated using the program Multiwfn [15]. The electrostatic potentials were calculated on the molecular surface, taking this to be the 0.001 a.u. contour of the electronic density [5]. The coefficients a, b, c, d, e, and f were determined from least-squares fitting to reliable experimental values of enthalpies of sublimation of 23 adamantanes (Table 1). These compounds were selected on the basis of comparison between experimental and calculated gas-phase enthalpies of formation [12]. For the first 15 compounds in Table 1, the difference between experimental and calculated values of $\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\circ}(\mathrm{g})$ does not exceed 5 kJ·mol^{-1}. Although this difference is larger for other compounds, the analysis of experimental data suggests that the discrepancy is due to errors in the $\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\circ}(\mathrm{cr})$ values rather than errors in the sublimation enthalpies. The sublimation enthalpies for six adamantanes considered in Ref. [12] (2-nitro-, 1,3-dinitro, 2,2-dinitro, 2-cyano-2-nitro-, 1-chloroadamntane, and 1,1′-diadamantyl ketone) were not included in the least-squares fitting because a fairly large discrepancy between the experimental and theoretical $\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\circ}(\mathrm{g})$ values could be due to both inaccuracies in the crystalline phase enthalpy of formation and sublimation enthalpy. The computed values of the descriptors involved in Eq. (3) and coefficients a, b, c, d, e, and f are given in Table S1 of Supplementary material.

The gas-phase enthalpy of formation of rimantadine was calculated from isodesmic reactions using G4 energies [29]. All quantum chemical calculations were performed with the Gaussian 16 package of programs [30].

3. Results and discussion

3.1. Sublimation enthalpy

Table 1 shows the comparison between the experimental sublimation enthalpies and those calculated by Eq. (3). It is seen that the difference is within only 4 kJ·mol^{-1} for all compounds, except for 1-aminoadamantane for which the calculated value is about 13 kJ·mol^{-1} larger than the experimental one. This is a rather unexpected result, because the difference between the calculated (−128.9 ± 3.0 kJ·mol^{-1}) [12] and experimental (−133.8 ± 2.4 kJ·mol^{-1}) [2] gas-phase enthalpies of formation of 1-aminoadamantane is much less, and this does not give grounds for assuming a large inaccuracy in the experimental value of sublimation enthalpy. Note that the largest discrepancy occurs also for 1-aminoadamantane if Eq. (2) is used to calculate the sublimation enthalpies (Table S1 of Supplementary material).

In order to confirm this surprising finding, we increased the number of compounds used to determine the coefficients of Eq. (3). In addition to adamantanes, 37 different compounds were used in extended MEP model. Among these are nitrogen substituted analogue of adamantane (hexamethylenetetramine), perhydroanthracenes with fused six-membered rings, bicyclic, aromatic and polycyclic compounds with different functional groups. As can be seen from Table S2 of Supplementary material, this model performs worse than the model with adamantanes only, however, the maximum deviation occurs again for 1-aminoadamantane.

Another interesting finding from the present work concerns the comparison of sublimation enthalpies for compound sets with different substituents. As seen from Table 2, the sublimation enthalpies for pairs of compounds with R = H and R = CH_3 and with R = OH and R = NH_2 are very nearly the same for both members of each pair, and the values for the second pairs are substantially larger than for the first pairs, except for 1-aminoadamantane. At the same time, the calculated $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{\circ}$ values fit into the overall trend. Fig. 1 shows that the observed trend in sublimation enthalpies correlates well with the change in the calculated electrostatic potentials. It is seen, that the electrostatic potential distribution is significant different for two pairs of compounds, what agrees with a large difference in the calculated values of σ_{tot}^2. The latter is an indicator of the variability and range of $V_S(\mathbf{r})$ over the entire molecular surface [6]:

$$\sigma_{\mathrm{tot}}^2 = \sigma_+^2 + \sigma_-^2 = \frac{1}{m}\sum_{i=1}^{m}[V_S^+(\mathbf{r}_i) - \bar{V}_S^+]^2 + \frac{1}{n}\sum_{j=1}^{n}[V_S^-(\mathbf{r}_j) - \bar{V}_S^-]^2$$

Therefore, one can expect from Fig. 1 that the $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{\circ}$ value of 1-aminoadamantane is rather closer to that of 1-adamantanol and differs from the sublimation enthalpy of adamantane.

Finally, sublimation and vaporization enthalpies of 1-aminoadamantane were also calculated by atomic group additivity method recently presented by Naef and Acree [33]. This method is based on a large and comprehensive collection of experimental vaporization and

Table 1
Calculated and experimental enthalpies of sublimation (kJ·mol^{-1}) at T = 298.15 K.

Compound		Calculation, this work	Experiment	Reference	Experiment – calculation
1	Adamantane	59.6	59.1 ± 0.9	[16]	−0.5
2	1-Methyladamantane	65.4	67.8 ± 1.3	[17]	2.4
3	2-Methyladamantane	65.5	68.2 ± 1.3	[17]	2.7
4	1,3-Dimethyladamantane	71.3	67.8 ± 1.3	[17]	−3.5
5	2,2-Dimethyladamantane	70.2	73.6 ± 1.3	[17]	3.4
6	1,3,5,7-Tetramethyladamantane	83.5	83.7 ± 1.3	[17]	0.2
7	1-Adamantanol	82.5	86.6 ± 0.6	[18]	4.1
8	2-Adamantanol	85.7	88.7 ± 2.5	[19]	3.0
9	1-Acetyladamantane	82.9	84.2 ± 0.6	[20]	1.3
10	1-Carbomethoxyadamantane	83.8	82.4 ± 0.6	[21]	−1.4
11	1-Aminoadamantane	75.1	61.7 ± 0.6	[2]	−13.4
12	1-Cyanoadamantane	73.2	77.0 ± 1.2	[22]	3.8
13	2-Cyanoadamantane	78.2	75.8 ± 1.1	[22]	−2.4
14	1-Adamantylcarboxamide	109.5	108.0 ± 0.5	[23]	−1.5
15	1,1′-Biadamantane	114.5	113.8 ± 1.4	[24]	−0.7
16	1,3,5-Trimethyladamantane	77.3	77.8 ± 1.3	[17]	0.5
17	2-Methyl-2-adamantanol	87.9	91.4 ± 0.3	[25]	3.5
18	2-Adamantanone	66.1	65.8 ± 0.6	[18]	−0.3
19	1-Adamantanecarboxylic acid	100.4	98.3 ± 1.8	[18]	−2.1
20	2-Adamantanecarboxylic acid	102.9	99.8 ± 1.8	[18]	−3.1
21	*N,N*-Dimethyl-1-adamantylcarboxamide	96.9	97.5 ± 0.3	[26]	0.6
22	1-Nitroadamantane	81.0	81.2 ± 2.0	[27]	0.2
23	5-(1-Adamantyl)tetrazole	123.6	126.8 ± 1.5	[28]	3.2

Table 2
Comparison of experimental sublimation enthalpies (kJ·mol^{-1}) at T = 298.15 K for selected methyl-, hydroxy-, and amino-substituted molecules.[a]

Compound	R = H	R = CH_3	R = OH	R = NH_2
1R-Adamantane	59.1 ± 0.9 (59.6)[b]	67.8 ± 1.3 (65.4)[b]	86.6 ± 0.6 (82.5)[b]	61.7 ± 0.6 (75.1)[b]
4R-C_6H_4-CH_3			73.1 ± 0.6	76.2 ± 0.3
4R-C_6H_4-C(O)OH	89.8 ± 0.4	97.6 ± 0.4	121.1 ± 0.4	118.0 ± 1.0
4R-C_6H_4-C(O)NH_2	103.1 ± 0.4	109.6 ± 0.3	129.7 ± 1.9	131.0 ± 1.2
1R-Naphthalene	71.7 ± 1.3	65.7 ± 0.9	93.3	88.1 ± 0.4
9R-Fluorene	88.6 ± 0.2	91.2 ± 0.4	108.3 ± 0.5	112.3 ± 0.4
8R-Quinoline			89.0 ± 1.4	93.3 ± 0.5

[a] References to experimental sublimation enthalpies are given in Table 1 for adamantanes and in Refs. [31,32] for other compounds.

[b] Value calculated by MEP model is given in parentheses.

sublimation data published by Acree and Chickos [31,32]. The calculated value of vaporization enthalpy of 1-aminoadamantane, as seen from Table 3, is in good agreement with the experimental result, whereas the sublimation enthalpy is about 20 kJ·mol^{-1} larger than the experimental value.

Besides 1-aminoadamantane, Gobble et al. [3] have determined the vaporization enthalpy of another adamantane-based pharmaceutical, α-methyl-1-adamantanemethylamine (rimantadine). The experimental value, 68.7 ± 3.7 kJ·mol^{-1}, is in good agreement with the 68.8 kJ·mol^{-1} estimated using group additivity method [33]. Just like for 1-aminoadamantane, the sublimation enthalpy estimated by group additivity and MEP models is substantially larger than the vaporization enthalpy (Table 3).

Thus, theoretical estimations are not consistent with the experimental sublimation enthalpy of 1-aminoadamantane. Taking into account a good agreement between the results of two experimental studies performed by two groups of experienced researchers [2,3], it is almost impossible to assume any errors in the experimental measurements. It is known that many adamantane derivatives form orientationally disordered, or plastic, crystals [34]. The phase transitions from the ordered crystal to the plastic crystalline phase were observed, for instance, for adamantane [16], methyladamantanes [34], 2-methyl-2-adamantanol [35], and 2-adamantanone [36]. As can be seen from Table 1, the experimental sublimation enthalpies for the above compounds agree well with the values estimated in this work. In comparison with these compounds, the powder pattern of 1-aminoadamantane at T = 298.15 K indicated approximately 50% crystallinity [3], and therefore the transition from the rigid solid (totally crystalline phase) to the plastic crystals was not observed in the experimental studies [2,3]. On the other hand, the MEP and group additivity models estimate the

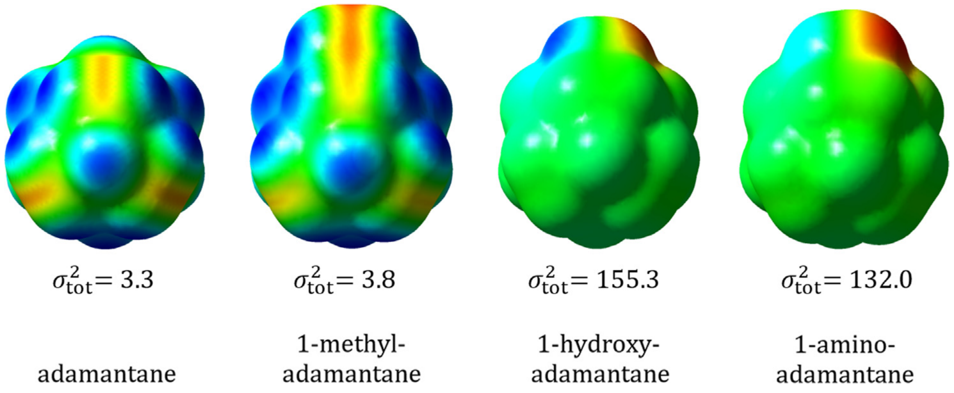
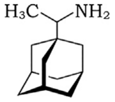


Fig. 1. Computed electrostatic potentials on the molecular density isosurfaces of adamantane and its derivatives. The red surface corresponds to a region of negative electrostatic potential, while the blue color corresponds to the positive potential. The values of σ^2_{tot} are given in (kcal·mol^{-1})^2. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 3
Experimental and theoretical enthalpies of sublimation and formation (kJ·mol^{-1}) of 1-aminoadamantane and α-methyl-1-adamantanemethylamine.

Compound	$\Delta_f H^\circ_m$(cr)	$\Delta^g_{cr} H^\circ_m$	$\Delta^g_{liq} H^\circ_m$	$\Delta_f H^\circ_m$(g)	Method	Reference
1-Aminoadamantane (Amantadine)	−195.4 ± 2.3	61.7 ± 0.6		−133.8 ± 2.4	Experiment	[2]
		~59.9 ± 3.5	59.9 ± 2.5		Experiment	[3]
		80.1	62.2		Group additivity	[33]
	−204.0 ± 7.0[a]	75.1 ± 5.0		−128.9 ± 3.0[b]	MEP, G4	This work
α-Methyl-1-adamantanemethylamine (Rimantadine)			68.7 ± 3.7		Experiment	[3]
		88.6	68.8		Group additivity	[33]
	−249.6 ± 7.0[a]	83.9 ± 5.0		−165.7 ± 3.6[c]	MEP, G4	This work

[a] Calculated using estimated values of $\Delta_f H^\circ_m$(g) and $\Delta^g_{cr} H^\circ_m$.
[b] Ref. [12].
[c] Calculated from isodesmic reactions using G4 energies (see Table S3 of Supplementary material).

total phase change enthalpies, and so the estimated sublimation enthalpy could be overestimated. Font and Muntasell [37,38] have studied the transitions from solid crystalline to plastic phase in pentaerythritols and have determined two values of sublimation enthalpy corresponding to crystalline and plastic phases. The values obtained for the solid crystalline phase were from 10 to 30 kJ·mol^{-1} higher than those for the plastic phase. The $\Delta^g_{cr} H^\circ_m$ values estimated in Table 3 by MEP and group additivity approaches are 13 and 18 kJ·mol^{-1}, respectively, higher than the experimental value. Thus, it is reasonable to suggest that the experimental value corresponds to the plastic crystal, whereas the theoretical values are estimated for totally crystalline phase.

3.2. Gas-phase enthalpy of formation

A simultaneous least-squares solution of isodesmic reaction network has allowed us to select 15 adamantanes with accurate experimental gas-phase enthalpies of formation [12]. For example, the theoretical value for adamantane, −132.0 ± 3.0 kJ·mol^{-1}, was in excellent agreement with the value of −132.3 ± 2.2 kJ·mol^{-1} determined in a very careful experimental study by Bazyleva et al. [16]. However, the $\Delta_f H^\circ_m$(g) value for 1-aminoadamantane obtained from isodesmic reaction network (−128.9 ± 3.0) kJ·mol^{-1} was 4.9 kJ·mol^{-1} larger than the experimental value (−133.8 ± 2.4) kJ·mol^{-1} [2]. Although this difference is within the combined errors of the two determinations, the computed value was suggested as more reliable. The reason for this preference is inconsistency of experimental $\Delta_f H^\circ_m$(g) value for 1-aminoadamantane with experimental enthalpies of formation for other adamantanes. This is also evident from the calculation of the enthalpy of formation of rimantadine (Table S3 of Supplementary material).

The enthalpy of formation of gas-phase rimantadine was calculated from 33 isodesmic reactions using 13 different adamantanes as reference species. The values obtained from these reactions range from −162.4 to −169.3 kJ·mol^{-1} and the mean value is −165.7 kJ·mol^{-1}. At the same time, 8 working reactions, where 1-aminoadamantane is selected as reference species, lead to enthalpies of formation of rimantadine in the range of more negative values (from −170.1 to −175.0 kJ·mol^{-1}) thus indicating that the experimental $\Delta_f H^\circ_m$(g) value for 1-aminoadamantane is somewhat underestimated.

3.3. Enthalpy of formation in crystalline phase

The values of $\Delta_f H^\circ_m$(g) and $\Delta^g_{cr} H^\circ_m$ estimated in this work give the enthalpy of formation of crystalline 1-aminoadamantane (Table 3) which is significantly more negative than the experimental value. Therefore, not only experimental sublimation enthalpy of 1-aminoadamantane but also experimental enthalpy of formation may be attributed to plastic crystal phase. It is possible that the study of totally crystalline pattern of 1-aminoadamantane will improve the agreement between experiment and theory. Using the calculated gas-phase enthalpy of formation and sublimation enthalpy, the enthalpy of formation of crystalline rimantadine is also estimated in this work (Table 3).

4. Conclusions

MEP model applied to adamantane and its derivatives shows a good agreement between the experimental and estimated sublimation enthalpies, with the exception of 1-aminoadamantane. However, the overestimation observed for the calculated sublimation enthalpy of 1-aminoadamantane may be explained assuming that the experimental value is determined for the plastic crystal, while the estimated value corresponds to the totally crystalline phase. In this case, we can say that the MEP model applied to a small group of structurally similar compounds may result in reliable estimates for sublimation enthalpies.

It is important to note that the sublimation enthalpies obtained for plastic crystals should be rejected from a set of experimental data used to fit the parameters of MEP model. Unfortunately, it is not always possible to understand the nature of phase transition observed in the published experimental measurements and this produces significant difficulties in developing a successful estimation method for sublimation enthalpy [32].

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.cplett.2018.09.044.

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