Lattice potential energy and standard molar enthalpy in the formation of 1–dodecylamine hydrobromide (1–$C_{12}H_{25}NH_3$·Br)(s)*

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This paper reports that 1-dodecylamine hydrobromide (1–$C_{12}H_{25}NH_3$·Br)(s) has been synthesized using the liquid phase reaction method. The lattice potential energy of the compound 1–$C_{12}H_{25}NH_3$·Br and the ionic volume and radius of the 1–$C_{12}H_{25}NH_3^+$ cation are obtained from the crystallographic data and other auxiliary thermodynamic data. The constant-volume energy of combustion of 1–$C_{12}H_{25}NH_3$·Br(s) is measured to be $\Delta_c U^o_m$(1–$C_{12}H_{25}NH_3$·Br, s) =–(7369.03±3.28) kJ·mol^{-1} by means of an RBC-II precision rotating-bomb combustion calorimeter at T=(298.15±0.001) K. The standard molar enthalpy of combustion of the compound is derived to be $\Delta_c H^o_m$(1–$C_{12}H_{25}NH_3$·Br, s)=–(7384.52±3.28) kJ·mol^{-1} from the constant-volume energy of combustion. The standard molar enthalpy of formation of the compound is calculated to be $\Delta_f H^o_m$(1–$C_{12}H_{25}NH_3$·Br, s)=–(1317.86±3.67) kJ·mol^{-1} from the standard molar enthalpy of combustion of the title compound and other auxiliary thermodynamic quantities through a thermochemical cycle.

Keywords: 1-dodecylamine hydrobromide, lattice potential energy, ionic radius, standard molar enthalpy of formation

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1. Introduction

Recently, as the energy crisis becomes increasingly serious, phase change materials (PCMs) are receiving more and more attention. Most traditional PCMs store or deliver energy by means of solid–liquid phase transitions.[1] Being types of solid–solid phase change materials (SSPCMs),[2,3] $(C_{12}H_{25}NH_3)_2MX_n$ {$(n = 4$ or 6), where M is a divalent or trivalent metal ion (M=Zn^{2+}, Cu^{2+}, Mn^{2+}, Cd^{2+}, Co^{2+}, etc.) and X is a negative haloid ion}, they have been extensively investigated in the past few decades as they show a variety of structural and magnetic phase transitions. They are characterized by high enthalpy and reversible solid–solid phase transitions between two polymorphic forms in the temperature range of 273–393 K. Furthermore, $(C_{12}H_{25}NH_3)_2MX_n$ can be directly processed into arbitrary shapes. Therefore, these new SSPCMs show great potential for their future use and currently new fields for their application are expanding rapidly. They may be applied effectively in fields such as solar energy utilization, waste heat recovery, energy-storage and so on. As one of the necessary intermediates or raw materials, 1–dodecylamine hydrobromide (1–$C_{12}H_{25}NH_3Br$) plays an important role in the formation of $(C_{12}H_{25}NH_3)_2MBr_n$ in which the $C_{12}H_{25}NH_3^+$ cation bonds with the MBr_n^{2-} anion through ionic bonds.[4]

In recent years, great attention has been paid to research involving 1–dodecylamine hydrobromide. Gordon *et al.* investigated the crystal structure and some properties of n-dodecylammonium bromide by x-ray diffractometer, automatic variable-temperature moving-film powder camera and single-crystal techniques in 1953.[5] In 1974, Lunden provided a three-dimensional single-crystal study of n-dodecylammonium bromide.[6] These studies focused on the crystal structure. However, some important thermodynamic data such as lattice potential energy, standard molar enthalpies of combustion and formation of the title compound have not been reported until now. This is needed in order to develop new application fields and to carry out relevant theoretical research. Lattice potential energy[7–9] is vital for the

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measurement of the bonding ability of the molecules or ions in the crystal structure, and its relationship with many significant physicochemical substance properties. The standard molar enthalpy of combustion of a substance is one of the most fundamental thermodynamic properties used when calculating a substance's standard molar enthalpy of formation and other thermodynamic data. Standard molar enthalpy of formation is one of the most important thermodynamic properties used to calculate enthalpy changes, equilibrium constants and theoretical yields of reactions in which the substance is involved. In addition, the standard molar enthalpy of formation of a substance is closely related to other physical, biological, physiological and chemical properties.[10]

Combustion calorimetry is often used to determine the standard molar enthalpies of formation of many important organic substances in industry and scientific research based on the data of enthalpies of combustion and some auxiliary thermodynamic quantities. The precision rotating-bomb combustion calorimeter is one of the basic devices necessary in some thermochemical research, and is especially useful for the determination of the combustion energies of some elements, organic compounds, metal organics, etc.[11] In this work, the lattice potential energy is calculated and the constant-volume energy of combustion ($\Delta_c U^o_m$) of 1–dodecylamine hydrobromide is determined using an RBC-II precision rotating-bomb combustion calorimeter. The standard molar enthalpies of combustion ($\Delta_c H^o_m$) and formation ($\Delta_f H^o_m$) of 1–dodecylamine hydrobromide are calculated.

2. Experimental section

2.1. Synthesis of 1–dodecylamine hydrobromide

The 1–dodecylamine and hydrobromic acid (≥ 40 mass %) chosen as the reactants and anhydrous ethyl alcohol used as the solvent were all of analytical grade. The reactants were weighed accurately at the molar ratio of $n(C_{12}H_{25}NH_2)$: n(HBr)=1:1, and slowly dissolved into the correct amount of anhydrous ethyl alcohol with sufficient stirring. The mixture was heated and stirred under reflux for 6 h. Thereafter the mixture was condensed by boiling off some of the liquid until a crystal membrane emerged on the surface of the solution. The final solution was naturally cooled to room temperature and filtered, and a colourless crystal was obtained. The product was re-crystallized three times with anhydrous ethyl alcohol and a colourless transparent crystal was produced. Finally, the sample was placed in a vacuum desiccator to dry in a vacuum at a temperature of 303.15 K for 6 h. The final product was put into a weighing bottle and preserved in a desiccator. The mass fraction purity of the compound was determined to be > 0.994 by high performance liquid chromatography (HPLC). The contents of the bromide in the compound were determined by chemical analysis. Elemental analysis (C, H, and N) was carried out on a Vario EL III CHNOS instrument made in Germany. These results showed that the mass fraction purity of the compound was > 0.994.

2.2. Rotating-bomb combustion calorimetry

The constant-volume energy of combustion of 1–dodecylamine hydrobromide was measured using a precision rotating-bomb combustion calorimeter (model: RBC-II type, made in Northwest University, China). The structure and principle of the calorimeter was described in detail in Ref. [12]. The initial temperature of the combustion reaction was automatically maintained at $T = (298.15 \pm 0.001)$ K. The uncertainty of the constant-volume energy of combustion results obtained from the calorimeter could reach $\pm 0.05\%$.

The sample was burned under an oxygen pressure of 2.5 MPa in the presence of 0.001 dm^3 of double-distilled water in the bomb to ensure equilibrium in the final state after combustion. The mole fraction purity of the oxygen used in the experiment was of research grade (> 0.99998). The mass of the sample was calibrated from air buoyancy on the basis of the determination of the density for a pellet of the sample. At $T = (298.15 \pm 0.001)$ K, the differential quotient of the constant-volume energy of combustion with the oxygen pressure, $(\partial U/\partial P)_T$, for the solid was assumed to be –0.2 $J \cdot g^{-1} \cdot MPa^{-1}$, a typical value for organic solids.[13]

The corrected value of the heat exchange between the calorimetric tube and its surroundings was calculated by means of the following equation according to the Linio–Pyfengdelel–Wsava formula:[12,13]

$$\Delta(\Delta T) = nV_0 + [(V_n - V_0)/(\overline{T_n} - \overline{T_0})] \cdot \left[(T_0 + T_n)/2 + \sum_{i=1}^{n-1} T_i - n\overline{T_0}\right], \quad (1)$$

where $\Delta(\Delta T)$/K denoted the corrected value of the heat exchange; n, the number of readings in the main

(or reaction) stage; V_0 and V_n/K·min^{-1}, the temperature drift rates in the initial and final stages, respectively (V was positive when the temperature decreased); $\overline{T_0}$ and $\overline{T_n}$/K, the average temperatures of the calorimeter during the initial and final stages, respectively; T_0 and T_n/K, the first and last readings of the main stage; $\sum_{i=1}^{n-1} T_i$, the sum of all the temperature readings of the main stage except for the last one; $(V_n - V_0)/(\overline{T}_n - \overline{T}_0)$, a constant related to the performance of the calorimeter.

After the experiment ended, the analytical methods used for the final products (gas, liquid, and solid) of the combustion reaction were the same as those in Ref. [12]. The combustion products were analysed mainly for carbon dioxide by the Rossini method.[13] No soot was observed in the sample crucible after each of combustion experiments. During the determination of the energy equivalent of the combustion calorimeter and measurements of the constant-volume energy of combustion of the sample, the mole ratio of real amounts of carbon dioxide produced in the combustion to the theoretical amounts were determined to be > 0.9992. This demonstrated that the combustion of the sample in the oxygen bomb was complete. Qualitative tests for CO with indicator tubes were negative within the limits of their sensitivity {mole fraction x (CO) $< 1{\cdot}10^{-6}$}. As a result, either carbon deposits or carbon monoxide formed during the combustion and the amount of NO_x in the final gas phase was negligible.

The energy equivalent of the calorimeter was determined from seven combustion experiments using benzoic acid with mole fraction purity (0.99998), which was purified three times by sublimation before use and its certified constant-volume energy of combustion $\Delta_c U = -26434$ J·g^{-1} at $T = 298.15$ K was recommended by National Institute of Standards and Technology (NIST). The energy equivalent of the combustion calorimeter was determined to be $\varepsilon = (18604.99 \pm 8.14)$ J·K^{-1} by the following formula under the same experimental conditions:[14]

$$\varepsilon = (Q \cdot W + q_c + q_N)/\Delta T, \tag{2}$$

where ε/(J·K^{-1}) was the energy equivalent of the calorimeter; Q/(J·g^{-1}), the energy of combustion of benzoic acid; W/g, the mass of benzoic acid; q_c/J, calibrated heat of combustion of wire {$q_c = G \cdot b$, in which G/(J·cm^{-1}) was the combustion enthalpy of Ni–Cr wire for ignition and $G = 0.9$ J·cm^{-1}; b/cm, the length of the actual Ni–Cr wire consumed in ignition}; q_N/J, correction value of total acid {$q_N = 5.97c$, in which 5.97/(J·mol^{-1}) was the enthalpy of solution and formation of nitric acid corresponding to 1 cm^3 of 0.1000 mol·dm^{-3} of sodium hydroxide solution; c/cm^3, the volume of the consumed 0.1000 mol·dm^{-3} sodium hydroxide solution}; ΔT/K, the corrected temperature rise of the combustion reaction. The calibration results from the energy equivalent of the rotating bomb combustion calorimeter are tabulated in Table 1.

Table 1. The calibration results from the energy equivalent of the rotating bomb combustion calorimeter, where W is the mass of benzoic acid; ΔT is the corrected temperature rise; q_N is corrected heat of total acid; q_c is the calibrated heat of the combustion wire; ε is the energy equivalent of the calorimeter.[a]

No.	W/g	ΔT/K	q_N/J	q_c/J	ε/(J·K^{-1})
1	0.98450	1.4004	25.90	12.60	18610.95
2	0.86320	1.2301	19.96	12.60	18576.04
3	1.10295	1.5658	19.49	12.60	18640.61
4	1.11940	1.5924	25.99	12.60	18606.39
5	0.82615	1.1764	23.82	12.60	18594.75
6	0.93520	1.3317	19.31	11.70	18586.83
7	0.84385	1.1999	22.46	12.60	18619.38
	$(\overline{x} \pm \sigma_a)$		$\varepsilon = (18604.99 \pm 8.14)$ J·K^{-1}		

[a] in which $\overline{x}$ is the mean value of a set of measurement results; $\sigma_a = \sqrt{\sum_{i=1}^{n} (x - \overline{x})^2/n(n-1)}$, n is the experimental number; x_i is a single value in a set of measurements.

In this work, after the experiment ended, the fittings and the inside wall of the bomb were washed using double-distilled water; then the washing solution was cooled to room temperature and transferred to a volumetric flask. The total amount of acid was obtained by titrating the solution to a phenolphthalein

end-point with 0.1000 mol·dm^{-3} sodium hydroxide solution. Because $C_{12}H_{25}NH_3$·Br(s) contains bromine and nitrogen, the final bomb-solution would contain HBr(aq) and HNO_3(aq). In the analysis, the total amount of HNO_3 is determined using the Devarda's alloy method.[12] The total amount of HBr(aq) in the solution is determined according to the difference between the total amount of acid and the amount of HNO_3(aq) in solution. The results demonstrate that the mole ratio of the real amount of HBr(g) produced in the combustion to the theoretical amount is determined to be > 0.9991.

3. Results and discussion

3.1. Lattice potential energy, ionic volume and ionic radius

Equation (3) used to estimate lattice potential energy of general type of salts M_pX_q is obtained from Ref. [9]

$$U_{\rm POT} = \sum n_i z_i^2 (\alpha'/V_{\rm m}^{1/3} + \beta'), \tag{3}$$

where α' and β' are appropriate fitted coefficients chosen according to the stoichiometry of the salt, n_i is the number of ions with a charge z_i in the formula unit and $V_{\rm m}$ is the molecular volume.

For the salts MX(1:1), MX_2(1:2) and M_2X (2:1), equation (3) is changed to:

$$U_{\rm POT} = |z_+|\,|z_-|\,v(\alpha'/V_{\rm m}^{1/3} + \beta'), \tag{4}$$

where z_+ and z are the respective charges on the cation and anion of the compound, v is the number of ions per molecule and equals $(p + q)$. In the case of the salts with a formula MX and a charge ratio (1:1) like 1–dodecylamine hydrobromide, $z_+ = 1$, $z_- = 1$, $p = 1$, $q = 1$, $v = 2$, $\alpha' = 117.3$ kJ·mol^{-1}·nm, $\beta' = 51.9$ kJ·mol^{-1}, and $V_{\rm m}$ is in unit of nm^3,[9]

$$V_{\rm m}/({\rm nm}^3) = M_{\rm m}/\rho N_{\rm A} = 1.66045 \times 10^{-3} M_{\rm m}/\rho, \tag{5}$$

where $N_{\rm A}$ is Avogadro's constant, 6.02245×10^{23} molecule·mol^{-1}. Thus, formula (4) is changed to[9]

$$U_{\rm POT} = \gamma(\rho/M_{\rm m})^{1/3} + \delta, \tag{6}$$

where the values of the constants for MX (1:1) are: $\gamma = 1981.2$ kJ·mol^{-1}·cm and $\delta = 103.8$ kJ·mol^{-1}. The density $\rho/({\rm g\cdot cm^{-3}})$ and molar mass $M_{\rm m}/({\rm g\cdot mol^{-1}})$ are obtained from crystal structure data of 1–dodecylamine hydrobromide in Table 2, ρ = 1.177 g·cm^{-3}, and $M_{\rm m} = 266.26$ g·mol^{-1}.[15] The $V_{\rm m}$ is calculated to be 0.3756 nm^3 according to Eq. (5), consequently, the lattice potential energy of the compound is determined to be $U_{\rm POT} = 428.95$ kJ·mol^{-1}, which reveals that the structure of 1–dodecylamine hydrobromide is stable.

In addition, for a salt of molecular formula M_pX_q,

$$V_{\rm m} = pV_+ + qV_-, \tag{7}$$

where V_- and V_+ are the volumes of the anion and cation, $p = 1$ and $q = 1$ for MX (1:1), V_- for Br^- is reported to be 0.0363 nm^3.[16] The V_+ (the volume of the cation 1–$C_{12}H_{25}NH_3^+$) is estimated to be 0.3394 nm^3 based on $V_{\rm m} = 0.3757$ nm^3. The ionic radius of the cation (r_+) of 1–dodecylamine hydrobromide can also be derived to be 0.4327 nm in terms of $V_+ = 4\pi r_+^3/3$ if the cation may be approximately seen as a sphere.

In comparison with the past work[17] for 1–dodecylamine hydrochloride (listed in Table 2), it can be seen that the ionic radius of the 1–$C_{12}H_{25}NH_3^+$ cation ($r_+ = 0.4327$ nm) of 1–dodecylamine hydrobromide almost agrees with that in 1–dodecylamine hydrochloride ($r_+ = 0.4289$ nm). However, the lattice potential energy of 1–dodecylamine hydrobromide ($U_{\rm POT} = 428.95$ kJ·mol^{-1}) is slightly smaller than that of 1–dodecylamine hydrochloride ($U_{\rm POT} = 433.47$ kJ·mol^{-1}). This is mainly due to the different volumes of Cl^- and Br^-. As we know, the volume of Br^- ($V_{Br^-} = 0.0363$ nm^3) is larger than that of Cl^- ($V_{Cl^-} = 0.0298$ nm^3). Therefore, the electrostatic force between the cation and anion for 1–dodecylamine hydrobromide is smaller than that for 1–dodecylamine hydrochloride; and the lattice potential energy of 1–dodecylamine hydrobromide is smaller than that of 1–dodecylamine hydrochloride.

Table 2. Lattice potential energy and ionic radius of the cation 1–$C_{12}H_{25}NH_3^+$ of the title compound.

compound	1–$C_{12}H_{25}NH_3$·Br	1–$C_{12}H_{25}NH_3$·Cl
$M_{\rm m}$/g·mol^{-1}	266.26	221.80
ρ/g·cm^{-3}	1.177	1.022
$V_{\rm m}$/nm^3	0.3756	0.3604
$U_{\rm POT}$/kJ·mol^{-1}	428.95	433.47
V(1–$C_{12}H_{25}NH_3^+$)/nm^3	0.3394	0.3306
r(1–$C_{12}H_{25}NH_3^+$)/nm	0.4327	0.4289

3.2. Constant-volume energy of combustion of the title compound

The method for determining the constant-volume energy of combustion of the sample is the same as

that used in the calibration of the calorimeter with benzoic acid. The constant-volume energy of combustion of the sample according to equation (2) can be calculated to be:

$$-\Delta_{\rm c}U = (\varepsilon \cdot \Delta T - q_{\rm c} - q_{\rm N})/W, \quad (8)$$

where $\Delta_{\rm c}U/({\rm J}\cdot{\rm g}^{-1})$ is the constant-volume energy of combustion of the sample; W/g is the mass of the sample; the physical meanings of other symbols are the same as those in Eq. (2).

The measured results of the constant-volume energies of combustion of 1–dodecylamine hydrobromide, $\Delta_{\rm c}U/({\rm J}\cdot{\rm g}^{-1})$, is indicated in Table 3. At T = 298.15 K, the differential quotient of the constant-volume energy of combustion with the oxygen pressure, $(\partial U/\partial P)_T = -0.2$ J·g^{-1}·MPa^{-1}.[13] Considering that the pressure in the oxygen-bomb in the combustion of the sample is corrected from 2.50 MPa to 0.1 MPa (standard pressure), $\Delta P \approx -2.49$ MPa, the change in the constant-volume energy of combustion $\Delta(\Delta_{\rm c}U)$ is calculated to be 0.50 J·g^{-1}. Therefore, the real constant-volume energy of combustion of the title compound is corrected to be $\Delta_{\rm c}U^{\rm o}_{\rm m}$ = $-(27676.56\pm12.31)$ J·g^{-1}+0.50 J·g^{-1} = $-(27676.06\pm 12.31)$ J·g^{-1} = $-(7369.03\pm3.28)$ kJ·mol^{-1} based on $\Delta_{\rm c}U$ (kJ·mol^{-1}) = $\Delta_{\rm c}U$(J·g^{-1})·M(g·mol^{-1})·10^{-3}.

Table 3. The measured results of the constant-volume energies of combustion of the title compound at T = 298.15 K, where W is the mass of the sample; $\Delta_{\rm c}U$ is the constant-volume energy of combustion of the title compound; the physical meanings of other symbols are the same as those in Table 1.

compound	No.	W/g	$\Delta_{\rm c}T$/K	$q_{\rm N}$/J	$q_{\rm c}$/J	$-\Delta_{\rm c}U$/J·g^{-1}
1–$C_{12}H_{25}NH_3$·Br	1	0.49365	0.7395	86.69	12.60	27669.60
	2	0.51980	0.7788	91.29	10.80	27678.87
	3	0.51225	0.7668	89.96	12.60	27650.07
	4	0.50440	0.7548	88.58	12.60	27640.50
	5	0.51735	0.7758	90.85	12.60	27699.43
	6	0.51235	0.7689	89.98	12.60	27720.89
	$(\overline{x}\pm\sigma_a)$		$\Delta_{\rm c}U = -(27676.56\pm12.31)$ J·g^{-1}			

3.3. Standard molar enthalpy of combustion of the title compound

The standard molar enthalpy of combustion of 1–dodecylamine hydrobromide, $\Delta_{\rm c}H^{\rm o}_{\rm m}$ refers to the enthalpy change of the following combustion reaction at T = 298.15 K and P = 100 kPa:

$$\begin{aligned} &1\text{–}C_{12}H_{25}NH_3\cdot Br(s) + 75/4O_2(g) \\ &= 12CO_2(g) + 27/2H_2O(l) + 1/2N_2(g) + HBr(l). \quad (9)\end{aligned}$$

The standard molar enthalpy of combustion of the sample can be derived from the constant-volume energy of combustion at T = 298.15 K by means of the following formula:[18,19]

$$\Delta_c H^{\rm o}_{\rm m} = \Delta_{\rm c}U^{\rm o}_{\rm m} + \Delta n \cdot RT, \quad (10)$$

$$\Delta n = \Sigma n_i({\rm products, g}) - \Sigma n_i({\rm reactants, g}), \quad (11)$$

where Σn_i is the total amount (in mole) of gas presented as products or reactants, Δn(1–$C_{12}H_{25}NH_3$·Br, s)=–25/4 mol, R = 8.314 J·K^{-1}·mol^{-1} and T = 298.15 K. The calculated standard molar enthalpy of combustion of 1–dodecylamine hydrobromide is derived to be $\Delta_{\rm c}H^{\rm o}_{\rm m}$(1–$C_{12}H_{25}NH_3$·Br, s)= $-(7384.52\pm3.28)$ kJ·mol^{-1}.

3.4. Standard molar enthalpy of formation of the title compound

The standard molar enthalpy of formation of 1–dodecylamine hydrobromide, $\Delta_{\rm f}H^{\rm o}_{\rm m}$(1–$C_{12}H_{25}NH_3$·Br, s), is calculated by designing a thermochemical cycle[18–20] according to Eq. (9) as follows:

$$\begin{aligned} &\Delta_{\rm f}H^{\rm o}_{\rm m}(C_{12}H_{28}N\cdot Br, s) \\ &= 12\Delta_{\rm f}H^{\rm o}_{\rm m}(CO_2, g) + 27/2\Delta_{\rm f}H^{\rm o}_{\rm m}(H_2O, l) \\ &\quad + \Delta_{\rm f}H^{\rm o}_{\rm m}(HBr, l) - \Delta_{\rm c}H^{\rm o}_{\rm m}(C_{12}H_{28}N\cdot Br, s), \quad (12)\end{aligned}$$

where $\Delta_{\rm f}H^{\rm o}_{\rm m}(CO_2,\ {\rm g})=-393.51\pm0.13$ kJ·mol^{-1},[21] $\Delta_{\rm f}H^{\rm o}_{\rm m}(H_2O,\ {\rm l}) = -285.83\pm0.04$ kJ·mol^{-1},[21] $\Delta_{\rm f}H^{\rm o}_{\rm m}$(HBr, l)=$-121.55$ kJ·mol^{-1}.[22]

The standard molar enthalpy of formation of the title compound can be derived to be $\Delta_{\rm f}H^{\rm o}_{\rm m}$(1–$C_{12}H_{25}NH_3$·Br, s)=$-(1317.86\pm3.67)$ kJ·mol^{-1}.

The standard molar enthalpies of combustion and formation of the title compound were derived from the specific energy of the combustion result. They are tabulated in Table 4.

Table 4. Standard molar energy and enthalpy of combustion and the standard molar enthalpy of formation of the title compound under study at $T = 298.15$ K and $P^{O} = 0.1$ MPa.

compound	$-\Delta_c U^{o}_{m}$/kJ·mol^{-1}	$-\Delta_c H^{o}_{m}$/kJ·mol^{-1}	$-\Delta_f H^{o}_{m}$/kJ·mol^{-1}
1–$C_{12}H_{25}NH_3$·Br	7369.03 ± 3.28	7384.52 ± 3.28	1317.86 ± 3.67

4. Conclusions

The crystal structure of 1–dodecylamine hydrobromide (1–$C_{12}H_{25}NH_3$·Br)(s) was measured using x-ray crystallography. The lattice potential energy of the compound 1–$C_{12}H_{25}NH_3$·Br, the ionic volume and ionic radius of 1–$C_{12}H_{25}NH_3^+$ cation were obtained. The standard molar enthalpies of combustion and formation of the title compound were reported.

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