ORIGINAL RESEARCH

CrossMark

Enthalpies of formation of diamantanes in the gas and crystalline phase: comparison of theory and experiment

Olga V. Dorofeeva [1] (ID) · Oxana N. Ryzhova [1]

Abstract

Gas-phase enthalpies of formation of diamantane and some of its derivatives were calculated from isodesmic reactions using adamantane as reference species. The G4 theory was applied to calculate the energies of all molecules involved in the isodesmic reactions. The sublimation enthalpies were predicted by the molecular electrostatic potential (MEP) model. Their values were computed from an equation that describes the relationship between the sublimation enthalpy and computed crystal density, and molecular surface area plus four quantities obtained from the surface electrostatic potential. The coefficients in this equation were determined earlier from least squares fitting to reliable values of sublimation enthalpy of 23 adamantanes. The enthalpy formation of diamantanes in the crystalline phase was estimated on the basis of calculated gas-phase enthalpies of formation and sublimation enthalpies. The difference between experimental and theoretical data and inconsistencies in available experimental data are discussed.

Keywords Diamantanes · Enthalpy of formation · Enthalpy of sublimation · Isodesmic reactions · Electrostatic potential

Introduction

Diamantane is the second member of the diamondoid family and is composed of two fused adamantane cages (Fig. 1). Diamondoids have been of great interest in recent years due to their role in nanotechnology, drug delivery, and medicine [1]. Although the enthalpy of formation ($\Delta_f H^\circ_{298}$) of crystalline adamantane was determined by different authors, a large scatter in the reported values did not give confidence in its accuracy for a long time. Only the relatively recent work of Bazyleva et al. [2] has provided reliable experimental data for this compound. Much less attention was paid to diamantane. The experimental enthalpies of formation of crystalline diamantane [3–5] reported in the 1970s differ by as much as 50 kJ/mol. Differences also exist in the sublimation enthalpy of diamantane (Table 1). Clark et al. [4–6, 12] have

determined the enthalpies of formation and sublimation of diamantanone and isomeric methyldiamantanes and diamantanols. There are no other values of $\Delta_f H^\circ_{298}(\text{cr})$ in the literature. The sublimation enthalpies were measured later for two diamantanols by Gunawan et al. [7] and, as can be seen from Table 1, the new $\Delta_{sub} H^\circ_{298}$ values are significantly lower than those determined by Clark et al. [6].

Since the high-level theoretical calculations were not performed for diamantane and its derivatives, it is interesting to evaluate the thermochemical properties of diamantanes using present-day computational chemistry methods and thus to assess the accuracy of experimental data. Recently, we have carried out similar calculations for adamantanes using isodesmic reaction network to calculate the gas-phase enthalpies of formation [14] and molecular electrostatic potential (MEP) model [15] to estimate the sublimation enthalpies. In comparison with adamantanes, there is not much experimental data available for diamantanes and they are less reliable and, because of this, the isodesmic reaction network does not provide a reasonable solution. Thus, the isodesmic reactions involving adamantane as a reference species were used in this work to calculate the gas-phase enthalpy of formation of all diamantanes. Note that a high accuracy experimental $\Delta_f H^\circ_{298}$ (g) value of adamantane (-132.3 ± 2.2 kJ/mol) [2] is in excellent agreement with the theoretical value obtained from

✉ Olga V. Dorofeeva
   dorofeeva@phys.chem.msu.ru

[1] Faculty of Chemistry, Lomonosov Moscow State University, 119991 Moscow, Russia
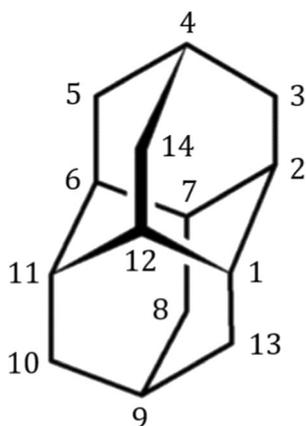
Fig. 1 Atom numbering for diamantane

isodesmic reaction calculations (− 132.0 kJ/mol), while the use of atomization reaction leads to much underestimated value (− 139.3 kJ/mol) [14].

In addition to diamantanes with available experimental data, the theoretical enthalpies of formation in the gas and crystalline phases were also calculated for three isomeric aminodiamantanes whose experimental data were not available in the literature.

Computational details

The gas-phase enthalpy of formation of diamantane was calculated using the isodesmic reaction:
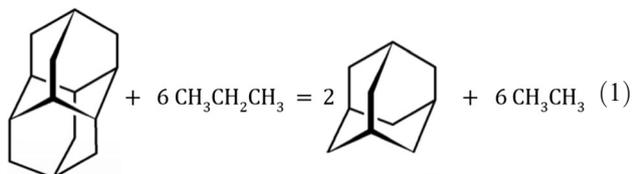
Similar reactions (Table S1 in the Supplementary data) were used to calculate the enthalpies of formation of diamantane derivatives. Note, that the reaction containing only cyclohexane-like structures
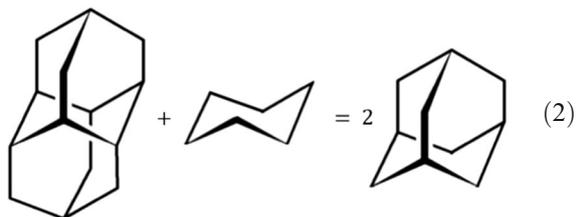
gives almost the same $\Delta_f H^\circ_{298}(g)$ value (− 155.9 kJ/mol) as that in Eq. 1 (− 156.1 kJ/mol). However, the reactions of this type for diamantane derivatives can lead to larger uncertainties because they include substituted adamantanes whose

enthalpies of formation are not so well established as the enthalpy of formation of adamantane. The enthalpies of all substances involved in isodesmic reactions were calculated at the G4 level of theory [16]. All quantum chemical calculations were performed using the Gaussian 16 package of programs [17].

The sublimation enthalpies of diamantanes were estimated by the MEP model using the equation proposed for adamantanes [15]. This equation describes the relationship between the sublimation enthalpy and computed crystal density (ρ), molecular surface area (A_S), and four quantities obtained from the surface electrostatic potential:

$$\Delta_{sub}H^\circ_{298} = a\rho + bA_S + c\bar{V}_S + d(\sigma^2_{tot}\nu) + e\Pi + f, \quad (3)$$

where $\bar{V}_S$ is the average value of the potential on the surface, σ^2_{tot} indicates the variability of the potential on the molecular surface and is equal 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 Π is the measure of local polarity. 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 [15]. For a set of 23 adamantanes, the $\Delta_{sub}H^\circ_{298}$ values predicted using the Eq. 3 produce a root-mean-square deviation (RMSD) of 3.7 kJ/mol.

The DFT/B3LYP/6-311++G(3df,2p) method was used to optimize geometries and determine the densities for generating the electrostatic potentials. All descriptors in Eq. 3 were calculated using the program Multiwfn [18]. Their values together with coefficients a, b, c, d, e, and f are given in Table S2 of Supplementary material. Figure 2 shows the computed electrostatic potentials for diamantane and its derivatives.

Results and discussion

Diamantane

The results of first two determinations of enthalpy of formation of crystalline diamantane, − 282.6 kJ/mol [3] and − 232.3 kJ/mol [4], were very different from each other. Later, Clark et al. [5] repeated the combustion experiments and obtained a new enthalpy of combustion value in good agreement with that determined in independent measurements by W.D. Good from the Bartlesville Energy Center. By weighing these two results, the value of − 240.4 ± 1.5 kJ/mol was recommended for enthalpy of formation of crystalline diamantane [5]. This value combined with the sublimation enthalpy of 95.9 kJ/mol [6] gives − 144.5 ± 1.7 kJ/mol for the gas-phase enthalpy of formation of diamantane.

It is seen from Table 1 that this value is remarkably different from that calculated in this work from Eq. 1 using

Table 1 Experimental and calculated enthalpies of formation and enthalpies of sublimation (in kJ/mol) of diamantane and its derivatives

Compound	$\Delta_f H^\circ_{298}(cr)$	$\Delta_{sub} H^\circ_{298}$	$\Delta_f H^\circ_{298}(g)$	Comment	Reference
Diamantane	-282.6 ± 1.8	117.1 ± 8.0	-165.5 ± 8.4	Exp	[3]
	-232.3 ± 2.3	95.9 ± 0.8 (319 K)	-136.4 ± 2.4	Exp	[4, 6]
	-241.8 ± 2.6	95.9 ± 0.8 (319 K)	-145.9 ± 2.7	Exp	[5]
	-240.4 ± 1.5[a]	95.9 ± 0.8 (319 K)	-144.5 ± 1.7	Exp, recommended	[5]
		92.1 ± 5.0		Exp	[7]
			$-138 \div 160$	Calc[b]	[5]
		75.3		Calc[c]	[8]
			-142.7	Calc[d]	[9]
		82.8		Calc, MEP[e]	[10]
		73.5		Calc, MEP[f]	[10]
		80.6		Calc, GA[g]	[11]
	-239.3	83.2	-156.1	Calc[h]	This work
1-Methyldiamantane	-247.4 ± 3.3	80.6 ± 0.4 (322 K)	-166.7 ± 3.6	Exp	[4–6]
		80.0		Calc, GA[g]	[11]
	-278.5	87.5	-191.0	Calc[h]	This work
3-Methyldiamantane	-260.4 ± 2.0	103.1 ± 1.0 (316 K)	-157.3 ± 2.4	Exp	[4–6]
			-166.0[i]	Est, recommended	[5]
		81.9		Calc, GA[g]	[11]
	-272.7	88.6	-184.1	Calc[h]	This work
4-Methyldiamantane	-261.5 ± 0.7	79.4 ± 1.3 (322 K)	-182.1 ± 1.3	Exp	[4–6]
		80.0		Calc, GA[g]	[11]
	-288.1	88.7	-199.4	Calc[h]	This work
Diamantan-1-ol	-428.8 ± 1.0	117.9 ± 0.6 (334 K)	-310.9 ± 1.2	Exp	[6, 12]
		102.1 ± 5.0		Exp	[7]
		97.9		Calc, GA[g]	[11]
	-444.3	101.9	-342.4	Calc[h]	This work
Diamantan-3-ol	-413.8 ± 1.5	116.1 ± 4.4 (338 K)	-297.6 ± 4.6	Exp	[6, 12]
		102.4		Calc, GA[g]	[11]
	-433.3	106.1	-327.2	Calc[h]	This work
Diamantane-4-ol	-435.0 ± 1.6	117.8 ± 0.2 (337 K)	-317.1 ± 1.6	Exp	[6, 12]
		108.8 ± 5.0		Exp	[7]
		97.9		Calc, GA[g]	[11]
	-445.5	103.3	-342.2	Calc[h]	This work
Diamantanone	-339.6 ± 1.6	103.1 ± 0.6 (320 K)	-236.5 ± 1.7	Exp	[12]
		88.8		Calc, GA[g]	[11]
	-351.2	89.8	-261.4	Calc[h]	This work
1-Aminodiamantane		89.2		Calc, GA[g]	[11]
	-242.7	94.2	-148.5	Calc[h]	This work
3-Aminodiamantane		84.6		Calc, GA[g]	[11]
	-231.2	94.5	-136.7	Calc[h]	This work
4-Aminodiamantane		89.2		Calc, GA[g]	[11]
	-247.8	96.6	-151.2	Calc[h]	This work

[a] Weighted average value based on two combustion enthalpies, see text for details

[b] Molecular mechanics calculations

[c] Atom-atom potential method

[d] Calculated from isodesmic reaction (Eq. 1) using B3LYP/6-31G(d) energies

[e] Molecular electrostatic potential (MEP) model; calculated using the equation $\Delta_{sub} H^\circ_{298} = a(A_S)^2 + b\sqrt{\sigma^2_{tot}\nu} + c$ from ref. [13]

[f] Calculated with equation from ref. [13] and coefficients a, b, and c determined using fitting for polycyclic saturated hydrocarbons at B3LYP/6-311++G (d,p) level of theory

[g] Group additivity (GA) method, calculated in this work using atom group contributions from ref. [11]

[h] Gas-phase enthalpy of formation is calculated from isodesmic reactions (Table 2) using G4 energies; sublimation enthalpy calculated by the MEP model (Eq. 3, DFT/B3LYP/6-311++G(3df,2p) method)

[i] Estimated value was recommended taking into account inconsistencies in experimental $\Delta_f H^\circ_{298}(g)$ values for methyldiamantanes and results of molecular mechanics calculations (see text for details)

G4 energies (-156.1 kJ/mol). The corresponding value computed earlier at the lower B3LYP/6-31G(d,p) level (-142.7 kJ/mol [9]) does not provide a confirmation of the accuracy of the experimental value because the DFT

calculations can give large errors even when applied to isodesmic reactions [19].

Three experimental values of sublimation enthalpy (117.1, 95.9, and 92.1 kJ/mol) were reported for diamantane, but the

Fig. 2 Computed electrostatic potentials on the molecular density isosurfaces of diamantane 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 $\sigma_{tot}^2 v$ are given in $(kcal/mol)^2$

$\sigma_{tot}^2 v = 0.46$ $\sigma_{tot}^2 v = 0.54$ $\sigma_{tot}^2 v = 0.51$ $\sigma_{tot}^2 v = 0.63$

diamantane   1-methyl-diamantane   3-methyl-diamantane   4-methyl-diamantane

$\sigma_{tot}^2 v = 18.7$ $\sigma_{tot}^2 v = 21.3$ $\sigma_{tot}^2 v = 17.9$ $\sigma_{tot}^2 v = 6.1$

diamantane-1-ol   diamantane-3-ol   diamantane-4-ol   diamantanone

$\sigma_{tot}^2 v = 11.1$ $\sigma_{tot}^2 v = 12.2$ $\sigma_{tot}^2 v = 11.5$

1-amino-diamantane   3-amino-diamantane   4-amino-diamantane
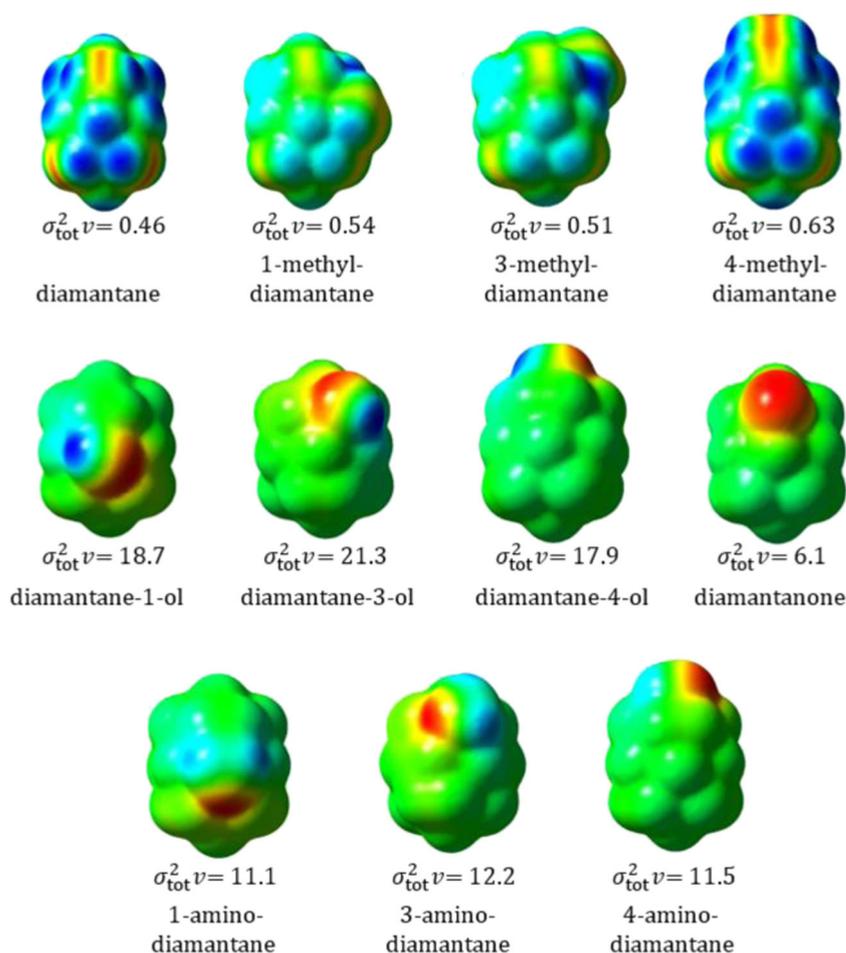
two of them were determined with large error (Table 1). The theoretical estimations by group additivity, atom-atom potential, and MEP models result in lower values from 73.5 to 83.2 kJ/mol (Table 1). Also, it should be noted that adding methyl group to adamantane (Table 2) increases the sublimation enthalpy, whereas the experimental $\Delta_{sub}H_{298}^{\circ}$ value of diamantane is, on the contrary, larger than that for 1- and 4-methyl substituted diamantanes (a too large value for 3-methyl diamantane seems to be unreliable). Since the calculations by the MEP model predict the sublimation enthalpies of

adamantanes in agreement with the experiment, it is reasonable to suggest the reliability of similar estimations for diamantanes. Table 2 also lists the $\sigma_{tot}^2 v$ parameters that are important in describing noncovalent interactions between molecules when representing properties such as enthalpies of sublimation [20]. It is seen that these values correlate with the change in sublimation enthalpies of adamantanes. A very similar trend is observed for diamantanes, and therefore we can suggest that experimental sublimation enthalpy of diamantane is significantly overestimated.

Table 2 Comparison of correlation between sublimation enthalpies in diamantane and adamantane and their methyl derivatives

Compound	$\Delta_{sub}H_{298}^{\circ}$ exp[a] kJ/mol	$\Delta_{sub}H_{298}^{\circ}$ calc[b] kJ/mol	$\sigma_{tot}^2 v$ calc[b] $(kcal/mol)^2$	Compound	$\Delta_{sub}H_{298}^{\circ}$ exp[c] kJ/mol	$\Delta_{sub}H_{298}^{\circ}$ calc[b] kJ/mol	$\sigma_{tot}^2 v$ calc[b] $(kcal/mol)^2$
Diamantane	95.9	83.2	0.46	Adamantane	59.1	59.6	1.86
1-Methyldiamantane	80.6	87.5	0.54				
3-Methyldiamantane	103.1	88.6	0.51	2-Methyladamantane	68.2	65.5	1.99
4-Methyldiamantane	79.4	88.7	0.63	1-Methyladamantane	67.8	65.4	2.12

[a] References to experimental data are given in Table 1

[b] This work, MEP model

[c] References to experimental data are given in ref. [14]

Fig. 3 Comparison of increments in $\Delta_f H^\circ_{298}(cr)$ for different substituent groups in adamantanes and diamantanes. Experimental data for adamantanes were taken from ref. [14]
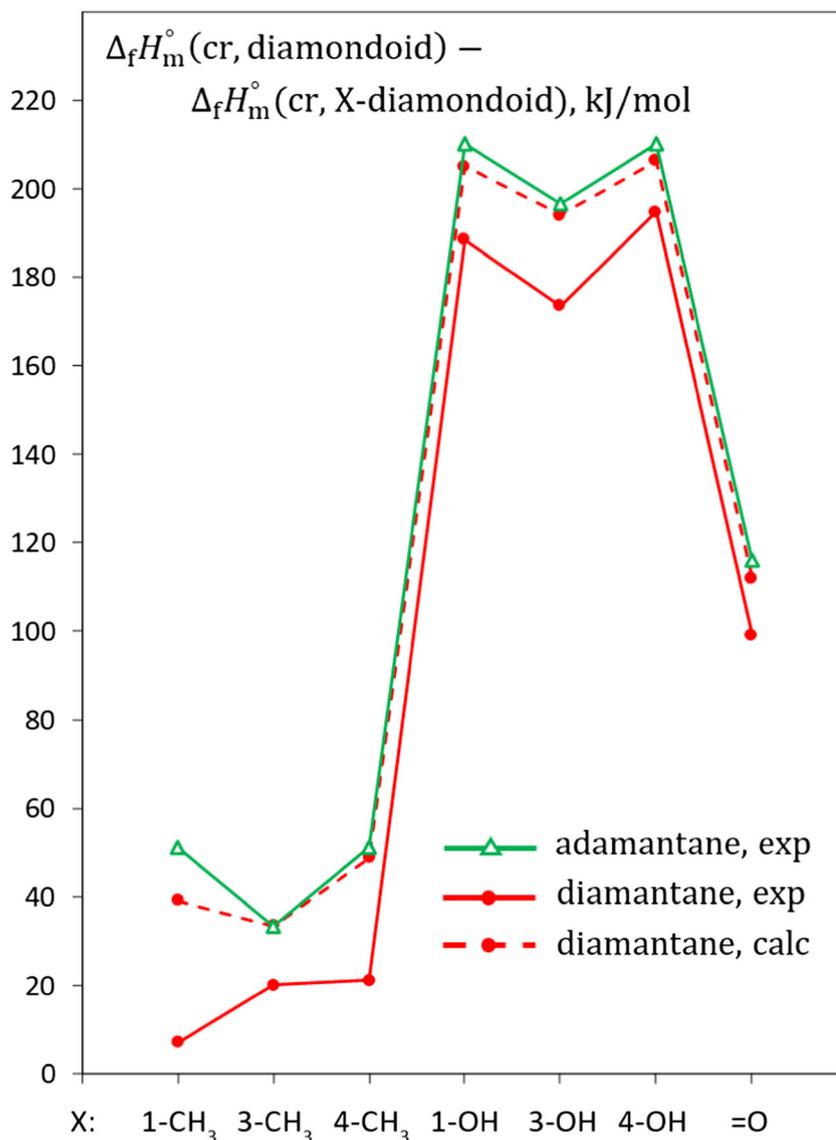
Assuming the sublimation enthalpy to be 83.2 kJ/mol, as estimated by the MEP model, and $\Delta_f H^\circ_{298}(g) = -156.1$ kJ/mol, as calculated from the isodesmic reaction (Eq. 1), we obtain the value of -239.3 kJ/mol for the enthalpy of formation of crystalline diamantane. As can be seen from Table 1, this value agrees well with the experimental value of -240.4 ± 1.5 kJ/mol [5] determined based on two independent measurements of combustion enthalpy. Thus, the theoretical determinations of this work seem to be quite reliable.

Diamantane derivatives

Experimental data on enthalpy of formation in crystalline phase and sublimation enthalpy were reported by Clark et al. [4–6, 12] for isomeric methyldiamantanes and diamantanols, as well as for diamantanone. As seen from Table 1, the experimental $\Delta_f H^\circ_{298}(cr)$ values are from 10 to 30 kJ/mol larger

than the theoretical values calculated in this work combining the estimated values of $\Delta_f H^\circ_{298}(g)$ and $\Delta_{sub} H^\circ_{298}$. However, the inconsistencies revealed in the $\Delta_f H^\circ_{298}(g)$ data for methyldiamantanes [5] denote inaccuracies in experimental data, at least for these compounds. Clark et al. [5] discuss the possible error in the enthalpy of combustion of 3-methyldiamantane and recommend the $\Delta_f H^\circ_{298}(g)$ value based on methyl group increments and molecular mechanics calculations rather than on experimental data.

In addition to data of Clark et al. [6], the sublimation enthalpy was determined for 1- and 4-diamantanol by Gunawan et al. [7]. These values, as seen from Table 1, agree well with the sublimation enthalpies estimated in this work, whereas the discrepancies with the data [6] are 9–16 kJ/mol. Note also that the sublimation enthalpies calculated by the MEP model are in good agreement with those estimated by the atomic group additivity method recently presented by Naef and Acree

[11]. This method is based on a large and comprehensive collection of experimental sublimation data published by Acree and Chickos [21, 22].

Considering additivity for $\Delta_f H^{\circ}_{298}(cr)$ values and assuming that experimental enthalpy of formation of crystalline diamantane [5] is accurate, it is interesting to compare the change in enthalpies of formation of adamantanes and diamantanes when the different groups are added to the unsubstituted molecules. The replacement of hydrogen atom in adamantane and diamantane by methyl, hydroxy, and carboxy groups leads to a decrease in enthalpy. This replacement in diamantane produces a structural change equivalent in thermochemical terms to that in adamantane (bridgehead positions 1 and 4 in diamantane can be considered equivalent to position 1 in adamantane, while the position 3 at secondary carbon in diamantane is equivalent to position 2 in adamantane). However, the corresponding group increments for diamantane and adamantane, as seen from Fig. 3, differ distinctly from each other. For example, replacement of hydrogen atoms in positions 1 and 2 in adamantane by a methyl group produces an experimental enthalpy increment of − 51 and − 33 kJ/mol, respectively, but the methyl group increments in diamantane (− 7, − 20, and − 21 kJ/mol in positions 1, 3, and 4) are much smaller. This discrepancy is unusually large for structurally similar compounds. On the other hand, Fig. 3 shows that –CH$_3$, –OH, and =O group increments in diamantane calculated in this work are in much better agreement with those in adamantane. This comparison provides additional support for the results of theoretical calculations.

Conclusions

The inconsistencies between experimental and theoretical enthalpies of formation and sublimation revealed in this work cannot be resolved with the existing data. It is known that diamantanes form orientationally disordered (or plastic) crystals [1, 23], and this creates difficulties in quantitative measurements and comparison of experimental and estimated values. If the sublimation enthalpy is determined for not totally crystalline phase, the estimated value can be overestimated as it was suggested for aminoadamantane [15]. However, as can be seem from Table 1, almost all theoretical sublimation enthalpies are lower than the experimental values.

The inconsistencies in experimental data for diamantanes noted in this work may be related to experimental uncertainties. Only for two diamantane derivatives, diamantan-1-ol and diamantan-4-ol, the sublimation enthalpy was determined twice and, as seen from Table 1, the difference between two results is large (16 and 9 kJ/mol, respectively). Also, there is no consistency in the experimental $\Delta_f H^{\circ}_{298}(g)$ values. Because of this, unlike in the case of adamantanes [14], we

were not able to get a reasonable solution for isodesmic reaction network by simultaneous adjustment of gas-phase enthalpies of formation of diamantanes.

As for theoretical calculations used in this work, their uncertainty may be larger than that for adamantanes [14, 15]. It was shown [14] that cyclohexane and fused cyclohexane rings (decalins and perhydroanthracenes), when used in isodesmic reactions as the reference species, lead to the underestimated $\Delta_f H^{\circ}_{298}(g)$ values of adamantane. A good agreement with the experiment was achieved only when using adamantane derivatives as references. Therefore, it cannot be ruled out that the more accurate results will be obtained if the diamantane derivatives are used in the working reactions instead of adamantane. New experimental studies are needed to validate predicting results from this work.

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

References

1. Mansoori GA (2007) Diamondoid molecules. Adv Chem Phys 136:207–258

2. Bazyleva AB, Blokhin AV, Kabo GJ, Charapennikau MB, Emel'yanenko VN, Verevkin SP, Diky V (2011) Thermodynamic properties of adamantane revisited. J Phys Chem B 115:10064–10072

3. Carson AS, Laye PG, Steele WV, Johnston DE, McKervey MA (1971) The enthalpy of formation of diamantane. J Chem Thermodyn 3:915–918

4. Clark T, Knox TM, Mackle H, McKervey MA, Rooney JJ (1975) Calorimetric evaluation of enthalpies of formation of some bridged-ring hydrocarbons. Comparison with data from empirical force field calculations. J Am Chem Soc 97:3835–3836

5. Clark T, Knox TM, McKervey MA, Mackle H, Rooney JJ (1979) Thermochemistry of bridged-ring substances. Enthalpies of formation of some diamondoid hydrocarbons and of perhydroquinacene. Comparisons with data from empirical force field calculations. J Am Chem Soc 101:2404–2410

6. Clark T, Knox T, Mackle H, McKervey MA, Rooney JJ (1975) Heats of sublimation of some cage hydrocarbons by a temperature scanning technique. J Chem Soc Faraday Trans 1(71):2107–2110

7. Gunawan MA, Poinsot D, Domenichini B, Dirand C, Chevalier S, Fokin AA, Schreiner PR, Hierso J (2015) The functionalization of nanodiamonds (diamondoids) as a key parameter of their easily controlled self-assembly in micro- and nanocrystals from the vapor phase. Nanoscale 7:1956–1962

8. Fyfe CA, Harold-Smith D (1975) Potential energy calculations of the rotational barriers in molecular solids. Part 3. – cage-like aliphatic molecules. J Chem Soc Faraday Trans 2 71:967–984

9. Fokin AA, Tkachenko BA, Gunchenko PA, Gusev DV, Schreiner PR (2005) Functionalized nanodiamonds. Part I. An experimental assessment of diamantane and computational predictions for higher diamondoids. Chem Eur J 11:7091–7101

10. Keshavarz MH, Zamani M, Atabaki F, Monjezi KH (2013) Theoretical investigation of phase transformations and molecular surface properties of polycyclic saturated hydrocarbon isomers of JP-10. Comput Theor Chem 1006:105–112

11. Naef R, Acree Jr WE (2017) Calculation of five thermodynamic molecular descriptors by means of a general computer algorithm based on the group-additivity method: standard enthalpies of vaporization, sublimation and solvation, and entropy of fusion of ordinary organic molecules and total phase-change entropy of liquid crystals. Molecules 22:1059

12. Clark T, Knox TM, McKervey MA, Mackle H (1980) Thermochemistry of bridged-ring substances. Enthalpies of formation of diamantan-1-, -3-, and -4-ol and of diamantanone. J Chem Soc Perkin Trans 2:1686–1689

13. Politzer P, Ma Y, Lane P, Concha MC (2005) Computational prediction of standard gas, liquid, and solid-phase heats of formation and heats of vaporization and sublimation. Int J Quantum Chem 105:341–347

14. Dorofeeva OV, Filimonova MA (2018) Self-consistent enthalpies of formation of adamantanes by isodesmic reaction network. J ChemThermodyn 126:31–37

15. Dorofeeva OV, Filimonova MA (2018) Sublimation enthalpy of 1-aminoadamantane: comparison of theory and experiment. Chem Phys Lett 711:231–235

16. Curtiss LA, Redfern PC, Raghavachari K (2007) Gaussian-4 theory. J Chem Phys 126:084108

17. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Petersson GA, Nakatsuji H et al (2016) Gaussian 16, (Revision B01). Gaussian Inc., Wallingford

18. Lu T, Chen F (2012) Multiwfn: a multifunctional wavefunction analyzer. J Comp Chem 33:580–592

19. Dorofeeva OV, Osina EL (2017) Performance of DFT, MP2, and composite ab initio methods for the prediction of enthalpies of formations of CHON compounds using isodesmic reactions. Comput Theor Chem 1106:28–35

20. Murray JS, Politzer P (1998) Statistical analysis of the molecular surface electrostatic potential: an approach to describing noncovalent interactions in condensed phases. J Mol Struct (THEOCHEM) 425:107–114

21. Acree Jr W, Chickos JS (2016) Phase transition enthalpy measurements of organic and organometallic compounds. Sublimation, vaporization, and fusion enthalpies from 1880 to 2015. Part 1. C_1-C_{10}. J Phys Chem Ref Data 45:033101

22. Acree Jr W, Chickos JS (2017) Phase transition enthalpy measurements of organic and organometallic compounds. Sublimation, vaporization, and fusion enthalpies from 1880 to 2015. Part 2. C_{11}-C_{192}. J Phys Chem Ref Data 46:013104

23. Clark T, Johnston DE, Mackle H, McKervey MA, Rooney JJ (1972) Diamantane derivatives, a new series of plastically crystalline compounds. The strain energy of diamantane. J Chem Soc Chem Commun:1042–1043