Energy Density of Adamantane-Containing Hydrocarbons in Condensed Phases

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Abstract—This paper provides an evaluation of the energy densities of adamantane-containing liquid hydrocarbons using an additive procedure we developed previously. Structural effects on the energy densities in these hydrocarbons are also discussed. The evaluated energy densities are compared to those for high-performance hydrocarbon jet fuels.

Keywords: adamantane-containing hydrocarbons, energy density, additive procedures, combustion enthalpies

INTRODUCTION

Petroleum fractions and some synthetic hydrocarbons have served as high-performance jet fuels because of their high energy density and other excellent physical and technical properties [1]. Hydrocarbons with small rings in their molecules, such as syntin (1-methyl-1,2-dicyclopropylcyclopropane), bicyclobutane, etc., have been considered to have the highest energy density due to high strain energy in their cycles [2, 3].

A monograph by Bagrii [4] cites various studies that have led to the assumption that the utilization of adamantane and its derivatives as jet fuels is infeasible due to low ring strain energy in adamantane moieties. Recently, a number of methods have been developed for the synthesis of alkyladamantanes and their mixtures with a density exceeding 0.9 g/cm^3, which presumably makes them suitable as components of high-density jet fuels [5, 6].

Our previous study demonstrates that the ring size of condensed hydrocarbons has no major effect on the mass enthalpy of combustion because the formation of each ring is accompanied by the loss of two hydrogen atoms [7].

The present paper investigated structural effects on energy density in essentially different adamantane derivatives, such as alkyl-, vinyl-, cyclopropyl-, phenyl-substituted and other derivatives. Various methods for synthesizing these compounds have been reported [4, 8], and efforts have been ongoing to improve existing methods and develop new ones [9]. However, calorimetric measurements of $\Delta_c H(T)$ have been performed only for adamantane and some methyladamantanes [10–16]. Therefore, we employed a simplified procedure to evaluate $\Delta_c H$ (298 K, $C_n H_m$) [7] for the substituted adamantane derivatives listed above.

Combustion Enthalpies of $C_n H_m$ Hydrocarbons with Various Structures

Table 1 summarizes the combustion enthalpies of adamantane and its alkyl derivatives.

The experimental gross (higher) enthalpies of combustion (i.e., those accounting for the formation of liquid water) of various hydrocarbons, $\Delta_c H^{\text{gross}}$ (298.15 K), were measured calorimetrically [11–19]. Based on these data, we calculated the net (lower) enthalpies of combustion, $\Delta_c H^{\text{net}}$ (298.15 K), by the following formula:

$$\Delta_c H^{\text{net}}(298.15\,\text{K}, C_n H_m) = \Delta_c H^{\text{gross}}(298.15\,\text{K}, C_n H_m)$$
$$+ \frac{m}{2}\Delta_{\text{vap}} H^{\circ}(298.15\,\text{K}, H_2 O), \qquad (1)$$

where $\Delta_{\text{vap}} H^{\circ}$ (298.15 K, $H_2 O$) is the enthalpy of water vaporization at 298.15 K, equal to 44.0 kJ/mol [19].

Table 1. Thermodynamic properties of alkyladamantanes and some hydrocarbon fuels in condensed phases

Compound, M, g/mol	T_{fus}, K	$\Delta_{fus}H\,(T_{fus})$, kJ/mol	d, g/cm^3	$-\Delta_c H^{gross}$, kJ/mol	$-\Delta_c H^{net}$, kJ/mol	$-\Delta_c H^{net}$, MJ/kg	$-\Delta_c H^{net}$, MJ/dm^3
Adamantane, $C_{10}H_{16}$, cr., 136.23	541.2 [21]	10.9 [21]	1.09 [10]	6029.2 [13]	5677.2	41.67	45.42
	543.2 [22]	13.8 [22]		6030.2 [12]	5678.2	41.68	45.43
				6032.3 [12]	5680.3	41.69	45.45
				6033.1 [14]	5681.1	41.70	45.45
				6033.4 [12]	5681.4	41.70	45.46
				6024.5 [15]	5672.5	41.64	45.39
1-Methyl adamantane, $C_{11}H_{18}$, cr., 150.26	392 [20]	3.71 [20]	1.06 [11]	6663.8 [13]	6267.8	41.71	44.22
				6658.4 [11]	6262.4	41.68	44.18
2-Methyl adamantane, $C_{11}H_{18}$, cr., 150.26	414.0 [20]		1.05 [11]	6684.3 [13]	6288.4	41.85	43.94
				6676.4 [11]	6280.4	41.79	43.89
2,2-Dimethyl adamantane, $C_{12}H_{20}$, cr., 164.29	416.2 [11]		1.01 [11]	7324.1 [11]	6884.1	41.90	42.32
1,3-Dimethyl adamantane, $C_{12}H_{20}$, liq., 164.29	245.0 [20]	0.92 [20]	1.10 [11]	7293.9 [11]	6854.0	41.72	45.89
	244.0 [23]	0.94 [23]		7317.7 [15]	6877.7	42.86	46.05
	247.8 [24]	1.54 [24]					
1-Ethyl adamantane, $C_{12}H_{20}$, liq., 164.29	225.6 [24]	11.28 [24]	0.935 [16]	7334.7 [16]	6894.7	41.97	39.24
1,3,5-Trimethyl adamantane, $C_{13}H_{22}$, liq., 178.31	253.6 [20]	1.73 [20]	1.08 [11]	7927.4 [11]	7443.4	41.74	45.08
				7952.6 [16]	7468.6	41.88	45.24
1,3,5,7-Tetramethyl adamantane, $C_{14}H_{24}$, cr., 192.34	337.2 [20]	9.82 [20]	1.12 [11]	8560.5 [11]	8032.5	41.76	46.77
				8577.0 [13]	8049.0	41.85	46.87
1,1′-Diadamantane, $C_{20}H_{30}$, cr., 270.45	561 [17]	70 [17]	1.14 [20]	11801.3 [17]	11141.3	41.19	46.93
Syntin, $C_{10}H_{16}$, liq., 136.23			0.851 [1]	6353.7 [18]	6006.41	44.1 [1]	37.50 [1]
Anthracene, $C_{14}H_{10}$, cr., 178.23			1.25 [1]	7061 [19]	7126.35	39.98 [1]	49.98 [1]
DAMST (di-2-methylstyrene), $C_{18}H_{20}$, cr., 236.35			1.078 [1]		9500.02	40.19 [1]	43.33 [1]
T-6, $C_{13.51}H_{25.39}$, liq., 187.51			0.841 [1]		8127.30	43.15 [1]	36.29 [1]

The mass and volumetric enthalpies of combustion (in MJ/kg and MJ/dm^3, respectively) were derived from the molecular weights (M) and densities (d) of the compounds under consideration [1, 10, 11, 16, 20] (see Table 1).

Among the nine compounds provided in Table 1, three adamantane derivatives (namely, 1,3-dimethyladamantane, 1-ethyladamantane, and 1,3,5-trimethyladamantane) are in the liquid phase at 298.15 K. However, in view of low fusion enthalpies of adamantane derivatives [17, 20–24] (below 1% of their combustion enthalpies), the differences in their physical state (i.e., crystal or liquid) can be disregarded for the purposes of the energy density of condensed alkyladamantanes.

At temperatures below 298.15 K, adamantane and some of its alkyl derivatives tend to form plastic crystals [25, 26]. This significantly decreases both the fusion enthalpies of these compounds and the density differences between their crystals and liquids. The plastic crystal temperature ranges of adamantane and its derivatives are illustrated in Fig. 1.

Table 1 clearly shows that the mass energy density of alkyladamantanes averages between 40 and 42 MJ/kg. Because most alkyladamantanes in condensed phases
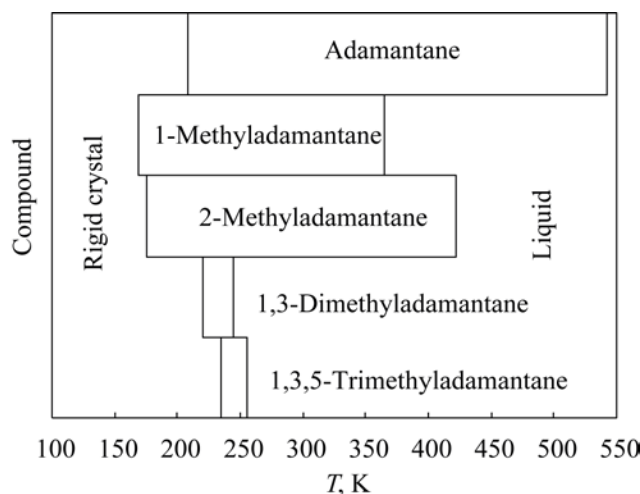
Fig. 1. Plastic crystal temperature ranges of adamantane and its derivatives.

where $\Delta_c H^{\text{net,gross}}$ (C) and $\Delta_c H^{\text{net,gross}}$ (H) are the contributions of C and H atoms, respectively, to the enthalpies of combustion of $C_n H_m$ hydrocarbons; E_i is the contribution of the strain energy of rings with $i = 2$ (double bond), 3, 4, 5, 6; E_{benz} is the strain energy of benzene (phenyl) moieties; and n_{benz} is the number of benzene (phenyl) moieties in the molecule.

For phenyl-free polycyclic $C_n H_m$ compounds, the number of rings can be evaluated as follows:

$$n_{\text{rings}} = \frac{2n + 2 - m}{2}. \tag{3}$$

The values of the constants in Eq. (2), required to determine the combustion enthalpies, were calculated from available experimental data on the gross molar enthalpy of combustion for 95 compounds differing in structure (including those with benzene moieties and condensed rings). The net enthalpies of combustion for these compounds were derived from Eq. (1).

Additive parameters (Table 2) can be used to calculate the gross and net molar enthalpies of combustion for hydrocarbons differing in structure; in this case, the calculation error (average difference between the calculated and experimental molar enthalpies of combustion) does not exceed about 0.4% [7].

In the present work, we utilized the data presented in Table 2 to calculate combustion enthalpies for a number of adamantane derivatives, as well as for some potential hydrocarbon fuels for which the experimental values of these properties are available. Thus, we were able to verify the additive methodology and assess its practicability for adamantane derivatives. The calculation results are summarized in Table 3.

The average difference between the calculated and experimental values of combustion enthalpy amounted to about 0.25%. This can be considered a satisfactory error for the simplified calculation procedure, thus proving the suitability of Eq. (2) for predicting hydrocarbon combustion enthalpies.

have a density above 0.9–1 kg/dm³, they exhibit a high volumetric energy density (39–46 MJ/dm³). In terms of mass or volumetric energy density, alkyl-adamantanes are comparable or even superior to high-performance hydrocarbon fuels such as syntin, anthracene, DAMST, and T-6. Among alkyladamantanes, 1,3,5,7-tetra-methyladamantane (solid), 1,1'-diadamantane (solid), and 1,3,5-trimethyladamantane (liquid) have the higher energy densities.

Prediction of Energy Density for Adamantane Derivatives

To date, no common procedure has been developed to search for high-energy-density compounds. In accordance with the additive procedure we proposed in reference [7] to calculate the molar enthalpy of combustion of hydrocarbon fuels, the gross and net enthalpies of combustion for compounds with various structures (including those with benzene moieties and condensed rings) can be estimated by the formula:

$$\Delta_c H^{\text{net,gross}}(C_n H_m) = n\Delta_c H^{\text{net,cross}}(C) + m\Delta_c H^{\text{net,gross}}(H)$$
$$+ \sum n_{\text{rings}} E_i^{\text{net,cross}} + \sum n_{\text{benz}} E_{\text{benz}}^{\text{net,cross}}, \tag{2}$$

Table 2. Additive constants for calculating gross and net enthalpies of combustion (kJ·mol⁻¹) for alkyladamantanes

Parameter	$-\Delta_c H$ (C)	$-\Delta_c H$ (H)	E_2	E_3	E_4	E_5	E_6	E_{benz}
$\Delta_c H^{\text{gross}}$	432.57	111.69	−50.67	−79.87	−76.87	1.63	31.5	35.37
$\Delta_c H^{\text{net}}$	432.57	89.69	−50.67	−79.87	−76.87	1.63	31.5	35.37

Table 3. Calculated gross enthalpies of combustion for adamantane derivatives and some hydrocarbon fuels at 298.15 K

Compound, M, g/mol	Calculation formula	$-\Delta_c H^{\mathrm{gross}}(C_n H_m)$, kJ/mol		Δ, kJ/mol	Δ, %
		experimental	calculated		
Adamantane, $C_{10}H_{16}$, cr., 136.23	$10\Delta_c H^{\mathrm{gross}}(C) + 16\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	6029.2 [13]	6018.2	11.0	0.18
		6032.3 [12]		12.0	0.20
		6032.3 [12]		14.1	0.23
		6033.1 [14]		14.9	0.25
		6033.4 [12]		15.2	0.25
		6024.5 [15]		6.3	0.10
1-Methyl adamantane, $C_{11}H_{18}$, cr., 150.26	$11\Delta_c H^{\mathrm{gross}}(C) + 18\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	6663.8 [13]	6674.2	10.4	0.15
		6658.4 [11]		15.8	0.24
2-Methyl adamantane, $C_{11}H_{18}$, cr., 150.26	$11\Delta_c H^{\mathrm{gross}}(C) + 18\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	6684.3 [13]	6674.2	10.1	0.15
		6676.4 [11]		2.2	0.03
2,2-Dimethyl adamantaneн, $C_{12}H_{20}$, cr., 164.29	$12\Delta_c H^{\mathrm{gross}}(C) + 20\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	7324.1 [11]	7330.1	6.0	0.08
1,3-Dimethyl adamantane, $C_{12}H_{20}$, liq., 164.29	$12\Delta_c H^{\mathrm{gross}}(C) + 20\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	7293.9 [11]	7330.1	36.2	0.50
		7317.7 [15]		12.4	0.17
1-Ethyl adamantane, $C_{12}H_{20}$, liq., 164.29	$12\Delta_c H^{\mathrm{gross}}(C) + 20\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	7334.7 [16]	7330.1	4.6	0.06
1,3,5-Trimethyl adamantane, $C_{13}H_{22}$, liq., 178.31	$13\Delta_c H^{\mathrm{gross}}(C) + 22\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	7927.4 [11]	7986.1	58.7	0.74
		7952.6 [16]		33.5	0.42
1,3,5,7-Tetramethyl adamantane, $C_{14}H_{24}$, cr., 192.34	$14\Delta_c H^{\mathrm{gross}}(C) + 24\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	8560.5 [11]	8642.0	81.5	0.95
		8577.0 [13]			
1,1′-Diadamantane, $C_{20}H_{30}$, cr., 270.45	$20\Delta_c H^{\mathrm{gross}}(C) + 30\Delta_c H^{\mathrm{gross}}(H) + 6E_6$	11801.3 [17]	11813.1	11.8	0.10
Syntin, $C_{10}H_{16}$, liq., 136.23	$10\Delta_c H^{\mathrm{gross}}(C) + 16\Delta_c H^{\mathrm{gross}}(H) + 3E_3$	6353.7 [18]	6352.3	1.4	0.02
Anthracene, $C_{14}H_{10}$, cr., 178.23	$14\Delta_c H^{\mathrm{gross}}(C) + 10\Delta_c H^{\mathrm{gross}}(H) + 3E_6$	7061.0 [19]	7066.8	5.8	0.08
	Average:			18.2	0.25

To investigate the dependence of the combustion enthalpies of adamantane derivatives on specific substituents using the above-mentioned additive procedure, we predicted the net molar enthalpies of combustion for a number of alkyladamantanes, dialkyladamantanes, trialkyladamantanes, cyclopropyladamantanes, and phenyladamantanes (Table 4). Although researchers have mentioned the synthesis of many such compounds [4, 8, 9], to date no experimental data on their properties have been reported.

The volumetric enthalpies of combustion of adamantane derivatives were calculated by the following equation:

$$\Delta_c H^{\mathrm{net}}(C_n H_m),\ \mathrm{MJ/dm^3}$$
$$= \frac{\Delta_c H^{\mathrm{net}}(C_n H_m),\ \mathrm{MJ/mol}}{V_m(C_n H_m),\ \mathrm{dm^3/mol}}. \quad (4)$$

The molar volumes of hydrocarbons were derived from the following equation [7]:

$$V_m(C_n H_m) = nV_m(C) + mV_m(H) + \sum n_i V_i + n_{\mathrm{benz}} \cdot V_{\mathrm{benz}}, \quad (5)$$

where $V_m(C)$ and $V_m(H)$ are the molar volumes of C and H atoms, respectively; V_i is the molar volume of an i-membered ring ($i = 2–6$); n_i is the number of i-membered rings ($i = 2–6$); and V_{benz} and n_{benz} are the molar volume and number of benzene moieties, respectively.

Taking into account the constants evaluated in [7], the molar volumes of hydrocarbons at 293 K can be derived with a mean error of about 0.9% from the following equation:

$$V_m(C_n H_m) = n(-16.62) + m6.41 + n_2 24.74 + n_3 22.89$$
$$+ n_4 20.00 + n_5 15.17 + n_6 12.08 + n_{\mathrm{benz}} 91.90. \quad (6)$$

Table 4. Predictive calculation of net enthalpies of combustion for substituted adamantane derivatives C_nH_m in condensed phases

Compound, M, g/mol	$-\Delta_cH^{net}(C_nH_m)$, kJ/mol	$-\Delta_cH^{net}(C_nH_m)$, MJ/kg	V_m, cm^3/mol	d, g/cm^3	$-\Delta_cH^{net}(C_nH_m)$, MJ/dm^3
n-Propyladamantane, $C_{13}H_{22}$, 178.31	7507.09	42.07	181.2	0.984	41.40
1,3-Dipropyladamantane, $C_{16}H_{28}$, 220.39	9337.94	42.37	229.8	0.959	40.63
n-Butyladamantane, $C_{14}H_{24}$, 192.34	8114.04	42.19	197.4	0.974	41.1
Vinyladamantane, $C_{12}H_{18}$, 162.27	6761.43	41.67	156.9	1.034	43.09
1,3-Divinyladamantane, $C_{14}H_{20}$, 188.31	7856.62	41.72	181.2	1.039	43.35
Allyladamantane, $C_{13}H_{20}$, 176.30	7373.38	41.82	173.1	1.018	42.6
1-Cyclopropyladamantane, $C_{13}H_{20}$, 176.30	7402.58	41.99	171.3	1.029	43.22
1,3-Dicyclopropyladamantane, $C_{16}H_{24}$, 216.36	8994.92	41.57	209.9	1.031	42.84
Cyclohexyladamantane, $C_{16}H_{26}$, 218.39	9127.06	41.79	209.1	1.044	43.66
1-Phenyladamantane, $C_{16}H_{20}$, 212.33	8585.05	40.43	190.4	1.115	45.08
1,3-Diphenyladamantane, $C_{22}H_{24}$, 288.43	11503.86	39.88	248.2	1.162	46.34
1,3,5-Triphenyladamantane, $C_{28}H_{28}$, 364.52	14422.67	39.57	306.1	1.190	47.12
1,3,5-Triadamantylbenzene, $C_{36}H_{48}$, 480.77	19594.14	40.76	390.0	1.232	50.24
1,1′-Diadamantane, $C_{20}H_{30}$, 270.45	11153.1	41.24	232.4	1.164	47.99
Diadamantylmethane, $C_{21}H_{32}$, 284.48	11765.05	41.36	248.6	1.144	47.33

Although it is difficult to physically interpret the numerical values of the constants in Eq. (6), especially that for V_m(C), all the V_i constant values are positive. In contrast, in the method earlier developed by Yarovoi to calculate the molar volumes of alkanes, negative values of $V_m(C_i–C_j)$ were obtained for a number of moieties [27].

The calculated values of the mass and volumetric net enthalpies of combustion for adamantane derivatives presented in Table 4 lead to a number of conclusions with regard to the prospects for their practical use as jet fuels.

For clarity, a comparison of the mass and volumetric net enthalpies of combustion for the tested fuels is illustrated in Fig. 2.

The data provided in Tables 1, 4 and Fig. 2 indicate that the molecular structures of adamantane and its derivatives have a fairly low effect on their mass enthalpies of combustion, which average about 41.5 MJ/kg. This average enthalpy exceeds the mass energy density of high-performance fuels such as anthracene (39.98 MJ/kg) and DAMST (di-2-methylstyrene) (40.19 MJ/kg) [1].

Adamantane-containing hydrocarbons in condensed phases generally have a density of $d_{20} \geq (0.9–1.0)$ kg/dm^3. This accounts for their fairly high volumetric energy density, specifically in the range of 39–50 MJ/dm^3 (according to our estimates, see Tables 1 and 4), which exceeds the volumetric energy density for fuels such as syntin (37.7 MJ/dm^3) and T-6 (36.3 MJ/dm^3) [1].

Thus, in terms of the most critical physical and technical properties—mass and volumetric energy densities—substituted adamantine derivatives are comparable or even superior to well-known high-performance hydrocarbon fuels.
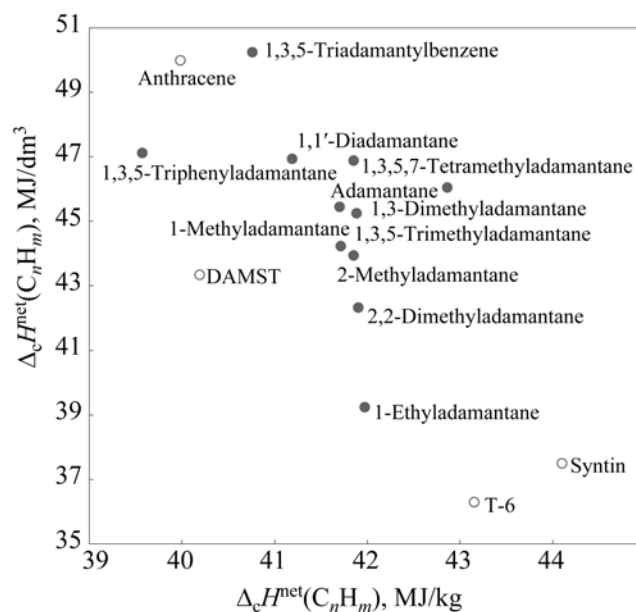

Fig. 2. Correlation between volumetric and mass combustion enthalpies for adamantine-containing compounds and hydrocarbon fuels: (●) adamantane and its derivatives; and (○) hydrocarbon fuels.

None of the hydrocarbon fuels exhibit high values of mass and volumetric energy density simultaneously (Fig. 2). We have no evident rationale for this fact. The priority of the energy density parameter—i.e., $\Delta_c H(T)$ MJ/kg or $\Delta_c H(T)$ MJ/dm^3—is likely governed by the specific performance characteristics of the fuel-based system under consideration.

To confirm the practicality of adamantane derivatives as jet fuels, due regard should also be given to other physical and technical properties: temperature and enthalpy of phase transition, saturated vapor pressure, heat capacity, ignition temperature, etc. [1]. The cost-benefit assessment of the industrial synthesis of these compounds is also of much importance [3].

CONCLUSIONS

The high mass and volumetric energy densities of adamantane-containing hydrocarbons provide sufficient reasons to regard them as potential jet fuels. Among these hydrocarbons, 1,3,5-trialkyladamantane, 1,1′-diamantane, 1,3,5-triphenyladamantane, and 1,3,5-triadamantylbenzene are the most promising for further detailed study.

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ACKNOWLEDGMENTS

CONFLICT OF INTEREST

The authors declare no conflict of interest requiring disclosure in this article.

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