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RESEARCH ARTICLE

Energy intensity of hydrocarbons in liquid and solid states

Gennady J. Kabo, Lubov A. Kabo, Larisa S. Karpushenkava[@], Andrey V. Blokhin

Belarusian State University, Minsk, 220030 Belarus
[@]Corresponding author, e-mail: karpushenkava@bsu.by

Abstract

Objectives. *The increased use of unmanned aerial vehicles necessitates the search for jet fuels based on hydrocarbon materials with high energy intensity and physical density. The purpose of the work was to analyze the influence of various factors on the mass energy intensity of hydrocarbons. This analysis is required to substantiate the algorithm for locating energy-intensive C_nH_m structures.*

Methods. *Combustion energy was calculated using additive procedures. The calculations were performed using Microsoft Excel.*

Results. *During the analysis of the mass energy intensity of C_nH_m hydrocarbons, the m/n ratio was discovered to be the decisive factor for achieving high values of the mass energy intensity of hydrocarbons. The energy intensity decreases when moving from alicyclic to cyclic hydrocarbons, and this decrease is not compensated by the production of strain energy. An additive scheme that allows the molar volume of hydrocarbons to be predicted with sufficient accuracy is proposed for calculating the volumetric enthalpies of combustion.*

Conclusions. *According to the thermodynamic analysis, n-alkanes have the highest mass energy intensities. The technology for extracting n-alkanes from oil fractions is well developed, and a decrease in the hydrogen content in the fuel results in a decrease in the mass energy intensity. It appears improbable that the mass and volumetric energy intensities of hydrocarbons seem will reach their maximum values simultaneously. Hydrocarbons that have a high m/n value, 2, 3, 4, 5, 6-membered rings, and phenyl fragments may have relatively high mass and volumetric energy intensities at the same time.*

Keywords: *hydrocarbon fuel, energy intensity, polycyclic hydrocarbons, mass enthalpy of combustion, volumetric enthalpy of combustion, additive calculations*

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НАУЧНАЯ СТАТЬЯ

Энергоемкость углеводородов в жидком и твердом состояниях

Г.Я. Кабо, Л.А. Кабо, Л.С. Карпушенкова[@], А.В. Блохин

Белорусский государственный университет, Минск, 220030 Беларусь
[@]Автор для переписки, e-mail: karpushenkava@bsu.by

Аннотация

Цели. *Расширение сфер использования беспилотных летательных аппаратов требует поиска реактивных топлив с высокой энергоемкостью и физической плотностью на основе углеводородных материалов. Цель работы заключалась в проведении анализа влияния различных факторов на массовую энергоемкость углеводородов, необходимого для обоснования алгоритма поиска энергоемких структур C_nH_m.*

Методы. *Энергия сгорания рассчитывались с использованием аддитивных процедур. Расчеты проводились в программе MS Excel.*

Результаты. *В ходе проведенного анализа массовой энергоемкости углеводородов C_nH_m было установлено, что решающим фактором для достижения высоких значений массовой энергоемкости углеводородов является отношение m/n. При переходе от алициклических углеводородов к циклическим энергоемкость снижается, и данное снижение не компенсируется возникающей энергией напряжения. Предложена аддитивная схема, позволяющая с достаточной точностью предсказать молярный объем углеводородов для расчета объемных энтальпий сгорания.*

Заключение. *Термодинамический анализ показал, что максимальной массовой энергоемкостью обладают н-алканы, технология извлечения которых из нефтяных фракций хорошо отработана, уменьшение же содержания водорода в топливе приводит к снижению массовой энергоемкости. Одновременное достижение максимальных значений массовых и объемных энергоемкостей углеводородов представляется маловероятным. Возможно, одновременно более высокой массовой и объемной энергоемкостью будут обладать углеводороды с высоким значением m/n, содержащие 2, 3, 4, 5, 6-ти членные циклы и фенильные фрагменты.*

Ключевые слова: *углеводородное топливо, энергоемкость, полициклические углеводороды, массовая энтальпия сгорания, объемная энтальпия сгорания, аддитивные расчеты*

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C_nH_m hydrocarbons in condensed states (liquid and crystal) are effective fuels for jet engines because of their high energy intensity and a set of other physical and technical characteristics [1]. The mass and volumetric enthalpies of combustion of hydrocarbons (Δ_cH (C_nH_m) MJ·kg^{-1}, Δ_cH (C_nH_m) MJ·dm^{-3}) are the key parameters for assessing the prospects of using hydrocarbons as fuel for air-jet engines. Technically, rocket engines that use fuels based on T-1 and T-6 petroleum fractions and synthetic hydrocarbons containing three- and four-membered cycles in the molecular structure have been implemented [2, 3]. The energy of strained C_3 and C_4 cycles in hydrocarbon molecules is generally accepted [2] to be released in the form of additional energy upon their combustion.

There are established methods for predicting the physicochemical properties of hydrocarbons based on the classical theory of molecular structure [4, 5]. However, there are no clearly formulated rules or algorithms for finding energy-intensive compounds. Therefore, the search for energy-intensive substances is carried out intuitively, and some commercially produced hydrocarbons, such as syntin (1-methyl-1,2-dicyclopropylcyclopropane) and bicyclobutane [6], do

not have maximum energy intensities although their synthesis methods and technologies are complex and expensive [3].

This paper presents an analysis of the influence of various factors on the mass energy intensity of hydrocarbons, which is necessary for substantiating a possible search algorithm for energy-intensive C_nH_m structures.

INFLUENCE OF DIFFERENT FACTORS ON THE MASS ENERGY INTENSITY OF C_nH_m HYDROCARBONS

It can be assumed a priori that the following, not in order of their importance, are the main factors that determine the energy intensity of fuels:

1. The state of hydrocarbons (crystal (cr.) or liquid (liq.)).

2. The elemental composition of C_nH_m, that is, the m/n ratio, or the mass fraction of hydrogen in the hydrocarbon.

3. The structural features of the C_nH_m molecules: the presence of double bonds and cycles of various sizes.

To study the influence of these factors on the mass energy intensity of C_nH_m we used the values of $\Delta_c H^{\text{gross}}$ (298.15 K, liq., cr.) of the gross (higher, standard) enthalpy of combustion of 95 C_6H_m–$C_{12}H_m$ hydrocarbons of various compositions and structures from the National Institute of Standards and Technology database (NIST, USA)[1] and their enthalpies of melting from reference books [7, 8]. The net (lower) heats of combustion were calculated using the following equation:

$$\Delta_c H^{\text{net}}(298.15\,\text{K}, C_nH_m, \text{liq., cr.}) = \Delta_c H^{\text{gross}}(298.15\,\text{K}, C_nH_m, \text{liq., cr.}) + \frac{m}{2}\Delta_{\text{vap}} H^{\circ}(298.15\,\text{K}, H_2O), \quad (1)$$

where the enthalpy of vaporization of water[1] $\Delta_{\text{vap}}H^0(298.15\text{ K}, H_2O) = 44.0\text{ kJ·mol}^{-1}$.

To determine the fraction of melting enthalpy in the enthalpy of combustion, the difference between the enthalpies of combustion of various hydrocarbons in the crystalline and liquid states was analyzed. The enthalpies of melting of hydrocarbons are significantly irregular, varying by a factor of 2–5 even among related compounds. This is largely determined by the existence of solid-phase transitions, including those associated with the formation of plastic crystals, in which the reorientation of molecules at the sites of crystal lattices is not excluded [9–11]. There are no simple correlations between the melting enthalpies and the melting point (T_{fus}) values such as Trouton's rule: $\frac{\Delta_{\text{fus}}H^{\circ}(T_{\text{fus}})}{T_{\text{fus}}} \neq \text{const}$. Estimates of the ratios $\frac{\Delta_{\text{fus}}H^{\circ}(T_{\text{fus}})}{\Delta_c H^{\circ}(298.15\text{ K})}$ for C_nH_m suggest that this value is within 0.1–0.5% in most cases and is comparable with the values of possible deviations $\Delta_c H^{\text{gross}}(C_nH_m)$ in measurements for samples of the same type from different authors. Thus, the mass energy intensity of C_nH_m can be assumed to be practically independent of the condensed state of the hydrocarbon: liquid or solid. However, the density of hydrocarbons, the volumetric energy intensity of fuels, and many other properties that influence the design of jet engines as well as their tactical and technical characteristics are all influenced by the state of substances.

The influence of the composition of C_nH_m hydrocarbons on the mass energy intensity was investigated based on the classical theory of molecular structure [4, 5]. It is worth noting that the value of the standard enthalpy of combustion increases as the mass fraction of hydrogen in molecules increases (Fig. 1). According to the Tatevskii principles of

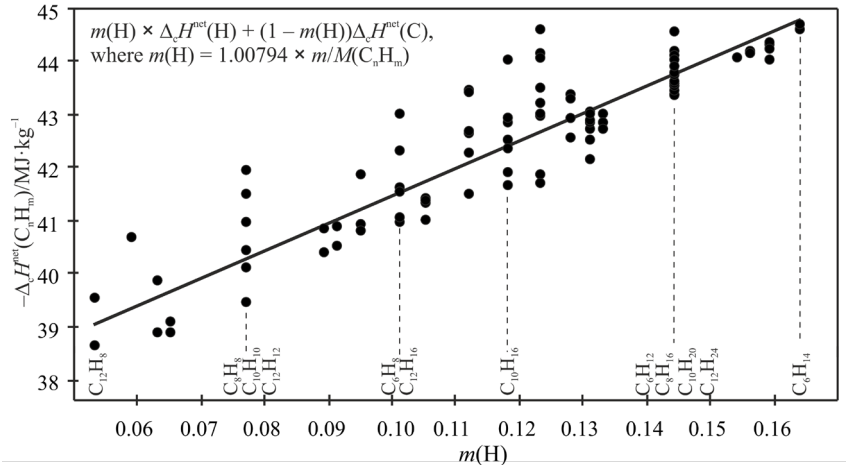


Fig. 1. Dependence of the mass enthalpy of combustion of hydrocarbons, $\Delta_c H^{\text{net}}(C_nH_m, 298.15\text{ K})$ MJ·kg^{-1}, on the mass fraction of hydrogen m(H) in the compound.

[1] NIST Chemistry Webbook. https://webbook.nist.gov/chemistry/. Accessed May 20, 2021.

classification of effective atoms [4, 5] the chemical individuality, i.e., the charge of nuclei determines the genus of atoms. Therefore, in a first approximation, the gross and net molar enthalpies of combustion of hydrocarbons can be represented as equation (2):

$$\Delta_c H^{\text{gross,net}}(C_nH_m, 298.15\ \text{K}, \text{kJ}\cdot\text{mol}^{-1}) = \\ = n\Delta_c H^{\text{gross,net}}(\text{C}) + m\Delta_c H^{\text{gross,net}}(\text{H}), \quad (2)$$

where n and m are the numbers of carbon and hydrogen atoms in the molecules, respectively; $\Delta_c H^{\text{gross,net}}(\text{C})$ and $\Delta_c H^{\text{gross,net}}(\text{H})$ are the fractions of the enthalpies of combustion attributed to the corresponding effective atoms. The numerical values of the additive contributions, $\Delta_c H^{\text{gross,net}}(\text{C})$ and $\Delta_c H^{\text{gross,net}}(\text{H})$ (kJ·mol^{-1}), were calculated using the least squares method from a system of 95 equations for $\Delta_c H°$ (C_nH_m, 298.15 K) borrowed from the NIST Chemistry Webbook of C_nH_m hydrocarbons (n = 6, 8, 10, and 12) with various m/n ratios, which suggests a variety of structural features of various classes of hydrocarbons, such as alkanes, alkenes, cycloalkanes, polycycloalkanes, and aromatic compounds. Although the choice of substances was rather arbitrary, substances with the smallest declared experimental error $\Delta_c H°$ (C_nH_m, 298.15 K) were shown preferences.

For mass enthalpies of combustion, the following equation is valid:

$$\Delta_c H^{\text{gross,net}}(C_nH_m, 298.15\text{K}) = m_C\Delta_c H^{\text{gross,net}}(\text{C})\ \text{MJ}\cdot\text{kg}^{-1} + \\ + m_H\Delta_c H^{\text{gross,net}}(\text{H})\ \text{MJ}\cdot\text{kg}^{-1}, \quad (3)$$

where m_C and m_H are the masses of the corresponding atoms in 1 kg (g) of the C_nH_m hydrocarbon, i.e., $m_C + m_H = 1$ kg (1 g).

The values of the additive contributions for the molar and mass enthalpies of combustion are presented in Table 1.

The deviation of the calculated $\Delta_c H^{\text{gross,net}}$ (C_nH_m) from the experimental values is $|\delta|_{\text{mean}} \approx 1.1\%$ on average. This difference exceeds $3 \times |\delta|_{\text{mean}}$ for 6 out of 95 hydrocarbons.

This indicates that predicting $\Delta_c H^{\text{gross,net}}$ (C_nH_m) based on the simplest qualification by the genus of effective atom is satisfactory. A comparison of the net mass enthalpies of combustion of well-characterized hydrocarbon fuels (Table 2) can provide additional confirmation of the efficiency of forecasting $\Delta_c H^{\text{gross,net}}$ (C_nH_m) based on equations (1) and (2).

Since the ratio of the atom contributions to the net mass enthalpy of combustion $\Delta_c H^{\text{net}}$ (C_nH_m, MJ·kg^{-1}) is $\Delta_c H^{\text{net}}(\text{H}) : \Delta_c H^{\text{net}}(\text{C}) = 87.977 : 36.275$, hydrocarbons with the highest values $\frac{m_H}{m_C}$ (with a larger mass fraction of hydrogen) should have the highest energy intensity (Fig. 1). This parameter varies from 0.335 for methane to 2.77×10^{-3} for fullerene hydride, $C_{60}H_2$.

All the noted regularities are practically independent of the state (liquid or crystal) of hydrocarbons, and no noticeable systematic deviation of C_nH_m in the solid state was observed in the calculations.

The influence of the molecular structure on the mass energy intensity of substances was determined according to the classical theory of molecular structure [4, 5]. According to the Tatevskii principles [4, 5], effective atoms in molecules are classified into species based on their valence states and nearest environment.

There are four species of effective carbon atoms in alkanes, depending on the first environment:

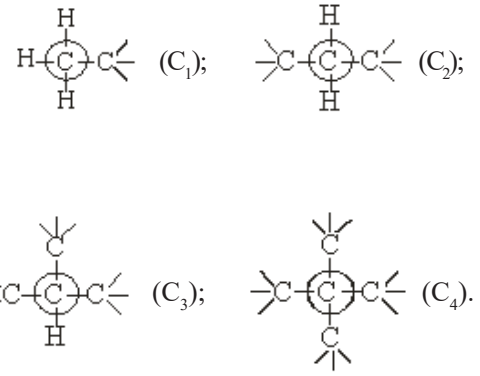


Table 1. Increments of the enthalpies of combustion of C and H atoms in C_nH_m hydrocarbons

$-\Delta_c H^{\text{gross}}$ (C), kJ·mol^{-1}	$-\Delta_c H^{\text{gross}}$ (H), kJ·mol^{-1}	$-\Delta_c H^{\text{net}}$ (C), kJ·mol^{-1}	$-\Delta_c H^{\text{net}}$ (H), kJ·mol^{-1}
435.687	110.675	435.687	88.675
$-\Delta_c H^{\text{gross}}$ (C), MJ·mol^{-1}	$-\Delta_c H^{\text{gross}}$ (H), MJ·mol^{-1}	$-\Delta_c H^{\text{net}}$ (C), MJ·mol^{-1}	$-\Delta_c H^{\text{net}}$ (H), MJ·mol^{-1}
36.275	109.83	36.275	87.977

Table 2. The net mass enthalpies of combustion of some hydrocarbon fuels

No.	Combustible C_nH_m	M, g·mol^{-1}	$\frac{m_H}{m_C}$	$-\Delta_c H^{net}$, MJ·kg^{-1}, exp.	$-\Delta_c H^{net}$, MJ·kg^{-1}, calc.
1	T-6 $C_{13.51}H_{25.34}$	187.5057	$\frac{0.136}{0.864}$	43.15*	43.30
2	α-Methylstyrene dimer $C_{18}H_{20}$	236.3514	$\frac{0.0853}{0.9147}$	40.2*	40.7
3	Anthracene $C_{14}H_{10}$	178.2292	$\frac{0.0566}{0.9434}$	39.9*	39.2
4	Toluene C_7H_8	92.1354	$\frac{0.0875}{0.9125}$	40.96*	40.8

* NIST Chemistry Webbook.

For calculating the gross enthalpies of combustion of alkanes (Table 3), Yarovoi [5] calculated the numerical values of the contributions $\Delta\Delta_c H^{gross}(C_i)$ of four species of effective atoms, C_i (i = 1–4). Table 3 also shows the values of similar additive increments calculated based on the results of this work using the following equation:

$$-\Delta\Delta_c H^{gross*}(C_i) = \Delta_c H^{gross}(C) + \\ +(4-i)\Delta_c H^{gross}(H), \quad (4)$$

where i is the species of effective atom (i = 1–4); $\Delta_c H^{gross}(C)$ is the increment of the enthalpy of combustion of the C atom (Table 1), and $\Delta_c H^{gross}(H)$ is the increment of the enthalpy of combustion of the H atom (Table 1).

The results of $\Delta\Delta_c H^{gross*}(C_i)$ calculations using equation (4) are in satisfactory agreement with the corresponding values obtained by Yarovoi [5] (Table 3).

This implies that the difference in the enthalpies of combustion of alkane isomers should be small. Indeed, the maximum values of the ratios of the enthalpy of isomerization to the enthalpy of combustion in condensed states are 0.43, 0.38, and 0.29% for hexane isomers, heptane, and octane, respectively [12]. In this case, *n*-alkanes are almost always characterized by the maximum enthalpy of combustion. Exceptions may exist for highly branched hydrocarbons with additional steric effects. For example, according to NIST, $\Delta_c H^{gross}$ (*n*-$C_{14}H_{30}$) = −9399.83 kJ·mol^{-1} and $\Delta_c H^{gross}$ (2,2,3,3,5,5,6-heptamethylheptane) = −9413.60 kJ·mol^{-1} ($\Delta\Delta_c H^{gross}$ ~0.15%).

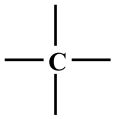
Thus, it is worth noting that the isomerism in alkanes and alkyl groups has a minor effect on the mass energy intensity of hydrocarbons.

The valence states and the "cyclicity" of effective carbon atoms affect the value of the enthalpy of combustion of hydrocarbons. We have shown [9, 13, 14] that introducing the "cyclicity" parameter of the effective atom, which is determined by the size and method of joining the cycles, results in the versatility of additive calculations of physicochemical properties. In this case, the number of types of effective carbon atoms increases to six:

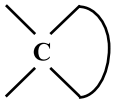
Table 3. Contributions of $\Delta\Delta_c H^{gross}(C_i)$ and $\Delta\Delta_c H^{gross*}(C_i)$ of the effective atoms to the enthalpy of combustion of alkanes

No.	Atom	$-\Delta\Delta_c H^{gross}(C_i)$, kJ·mol^{-1} [5]	$-\Delta\Delta_c H^{gross*}(C_i)$, kJ·mol^{-1}, this work	$\lvert\delta\rvert_{mean}$, %
1	C_1	770.45	767.71	0.36
2	C_2	645.98	657.04	0.31
3	C_3	535.51	546.36	1.27
4	C_4	421.32	435.69	3.4

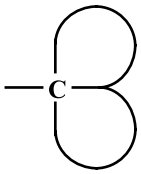
C – acyclic



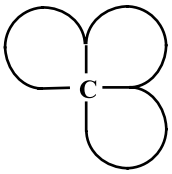
$C^{C^{I}}$ – monocyclic



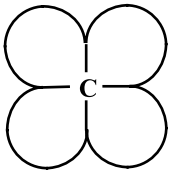
$C^{C^{I},C^{II}}$ – bicyclic



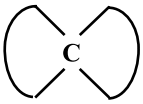
$C^{C^{I},C^{II},C^{III}}$ – tricyclic



$C^{C^{I},C^{II},C^{III},C^{IV}}$ – tetracyclic



$C^{S-C^{I},C^{II}}$ – spirocyclic



Conventionally, double bonds are considered two-membered cycles. Naturally, such a classification of effective atoms significantly increases the number of required additive constants. The possibility of predicting the enthalpy of combustion $\Delta_c H^{gross}$ (C_nH_m, 298.15 K) can be simplified using the generalized parameters of cycle strain energy, which are determined for monocyclic compounds as

$$E_i = \Delta_c H^{gross}(C_nH_m)_{exp.} - \Delta_c H^{gross}(C_nH_m)_{calc.} \quad (5)$$

In this ratio, $\Delta_c H^{gross}(C_nH_m)_{calc.}$ is calculated using the corresponding contributions for unstrained compounds in the state of ideal gas according to Benson [15] or Tatevskii and Yarovoi [4, 5]. Kozina [16] and Kolesov [17] studied the strain energies of cyclic hydrocarbons in detail. In [16], the conditionality of the E_i value was rightly noted, and in [17], E_i was demonstrated to be less dependent on the number of alkyl substituents in cyclic compounds. Table 4 presents the numerical values of E_i in cyclic compounds in the state of ideal gases.

We used equations similar to equation (5) to calculate the conditional strain energy (E_i^*) for monocyclic hydrocarbons in the liquid state:

$$E_i^*(kJ\cdot mol^{-1}) = \Delta_c H^{gross}(C_nH_m)_{liq.,\,exp.} - \Delta_c H^{gross}(C_nH_m)_{liq.,\,calc.} \quad (6)$$

Using the data in Table 1, the calculated value of the enthalpy of combustion of liquid hydrocarbons $\Delta_c H^{gross}(C_nH_m)_{liq.,\,calc.}$ was determined using equation (7). The fact that the increments for the liquid and crystalline states are practically indistinguishable in magnitude was considered:

$$\Delta_c H^{gross}(C_nH_m, kJ\cdot mol^{-1})_{liq.,\,calc.} = n\Delta_c H^{gross}(C)_{liq.} + m\Delta_c H^{gross}(H)_{liq.} \quad (7)$$

The results of E_i^* calculation and the change in the strain energy of the cycle during the transition from liquid to gaseous state are provided in Table 4.

The effective strain energies of the liquid hydrocarbon cycles are 35–45 kJ·mol^{-1} lower than those of the compounds in the ideal gas state. Five- and six-membered compounds are even more stable than their acyclic counterparts. The notable effects of energy stabilization of cyclic compounds in the liquid state are most likely associated with processes that result in an increase in the density of liquids due to a decrease in the intrinsic volume of molecules and an increase in intermolecular interaction.

As each new cycle or double bond is formed, the compound loses two hydrogen atoms. This causes a 2 × (–110.675) kJ·mol^{-1} (Table 1) decrease in the molar energy intensity, which is not compensated by the cycle strain energy even in the case of the most strained cyclopropane hydrocarbons (Table 4).

The strain energy of cycles for polycyclic compounds (E_i^{**}, Table 5) can differ significantly from that for monocyclic compounds (Table 4).

For polycyclic C_nH_m compounds, the number of cycles can be determined as

$$n_{i,cycle} = \frac{2n+2-m}{2}, \quad (8)$$

and the molar gross heat of combustion can be calculated as

$$\Delta_c H^{gross}(C_nH_m) = n\Delta_c H^{gross}(C) + m\Delta_c H^{gross}(H) + \sum_{i=2}^{6} n_{i,\,cycle} \times E_i^{**}, \quad (9)$$

where E_i^{**} is the effective strain energy for cycles i = 2, 4, 5, and 6 in the liquid state. The net heat of combustion is calculated in a similar manner.

Based on equation (9), new values of the additive constants, $\Delta_c H^{gross,net}(C)$ and $\Delta_c H^{gross,net}(H)$, $E_i^{**gross,net}$,

Table 4. E_i strain energies and E_i* effective (conventional) strain energies of cyclic hydrocarbons [13, 16]

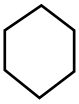
No.	Cycle type	E_i, id. gas, kJ·mol^{-1}	E_i^*, liquid, kJ·mol^{-1}	$\Delta_{gas}^{liq}E_i$, kJ·mol^{-1}
1		−93.5	−47.9	45.6
2		−115.5	−80.1	35.4
3		−111.3	−67.5	43.8
4		−25.1	9.3	34.4
5		−0.8	34.3	35.1

Table 5. Increments for $\Delta_c H^{gross,net}$ (298.15 K) values calculation

$\Delta_c H^{gross,net}$ (298.15 K)	kJ·mol^{-1}		MJ·kg^{-1}	
	gross	net	gross	net
$-\Delta_C H$(C)	432.57	432.57	36.87	36.87
$-\Delta_C H$(H)	111.69	89.69	106.16	84.33
E_2^{**}	−50.67	−50.67	−1.81	−1.81
E_3^{**}	−79.87	−79.87	−1.90	−1.90
E_4^{**}	−76.87	−76.87	−1.37	−1.37
E_5^{**}	1.63	1.63	0.023	0.023
E_6^{**}	31.50	31.50	0.374	0.374
$E_{benz.}^{**}$	35.37	35.37	0.453	0.453

(Table 5) were calculated using the least squares method. This allowed the calculation error to be reduced on average to $|\delta|_{mean}$ = 0.4% for all 95 compounds in the working database.

When calculating additive constants E_i^{**}, MJ·kg^{-1} (kJ·g^{-1}), it was assumed that

$$E_i^{**}(\text{MJ}\cdot\text{kg}^{-1}) = \frac{E_i^{**}(\text{kJ}\cdot\text{mol}^{-1})}{M(\text{CH}_2)\cdot i}, \quad (10)$$

and thus, for the benzene (phenyl) ring, it was determined as

$$E_{benz.}^{**}(\text{MJ}\cdot\text{kg}^{-1}) = \frac{E_{benz.}^{**}(\text{kJ}\cdot\text{mol}^{-1})}{M(\text{C}_6\text{H}_6)}. \quad (11)$$

The effectiveness of Equation (9) is illustrated by the calculation of the energy intensity of 11 $C_{10}H_{16}$ substances (Table 6). The calculated values of enthalpies of combustion were obtained using the data from Table 5. The mean calculation error was 0.34%, which is considered a good result for a simple additive procedure.

Equation (9) can also be used to calculate $\Delta_c H^{gross}(C_nH_m)$ of cage hydrocarbons with convex polyhedron structures using the Euler formula for calculating the number of facet cycles:

$$n_{cycle} = n_{ij} - n + 2, \quad (12)$$

where n_{ij} is the number of C–C bonds (edges), n is the number of atoms (vertices), and n_{cycle} is the number of cycles (faces).

Table 6. Experimental and calculated values of the gross enthalpy of combustion ($-\Delta_c H^{gross}$, kJ·mol^{-1}) of $C_{10}H_{16}$ hydrocarbons

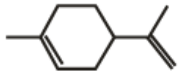
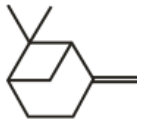
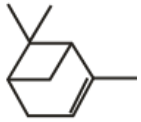
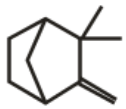
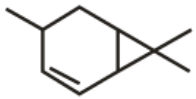
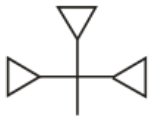
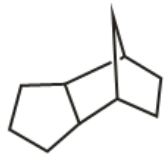
No.	Compounds		$-\Delta_c H^{gross}$, exp.[1]	Calculations		$-\Delta_c\Delta^{calc.}_{exp.} H^{gross}$	
				Equation	$-\Delta_c H^{gross}$	kJ·mol^{-1}	|δ|, %
1	*trans*-1-Methyl-1,2 dicyclopropyl-cyclopropane (syntin), liq.		6353.7 [18]	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+3E_3^{**}$	6352.4	1.4	0.02
2	Adamantane, cr.		6033.1	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+3E_6^{**}$	6018.2	14.9	0.25
3	Limonene, liq.		6128.3	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+2E_2^{**}+E_6^{**}$	6182.6	−54.3	0.89
4	α-Pinene, liq.		6205.0	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+E_2^{**}+E_4^{**}+E_6^{**}$	6208.8	−3.8	0.06
5	β-Pinene, liq.		6214.1	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+E_2^{**}+E_4^{**}+E_6^{**}$	6208.8	5.3	0.09
6	Camphene, cr.		6146	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+E_2^{**}+2E_5^{**}$	6160.2	−14.2	0.23

Table 6. Continued

No.	Compounds		$-\Delta_c H^{gross}$, exp.[1]	Calculations		$-\Delta_c\Delta^{calc.}_{exp.} H^{gross}$	
				Equation	$-\Delta_c H^{gross}$	kJ·mol^{-1}	|δ|, %
7	3-Carene, cr.		6192.2	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+E_2^{**}+E_3^{**}+E_6^{**}$	6211.8	−19.6	0.32
8	Tricyclene, cr.		6146.7	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+E_3^{**}+2E_5^{**}$	6189.4	−42.7	0.69
9	Perhydrotriquinacene, cr.		6062.8	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+3E_5^{**}$	6107.9	−45.1	0.74
10	Tricyclopropylmethane, liq.		6380.8	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+3E_3^{**}$	6352.4	28.5	0.45
11	4,7-Methano-1H-indene, octahydro-, cr.		6109	$10\Delta_c H^B(C)+16\Delta_c H^B(H)+3E_5^{**}$	6107.9	1.1	0.02
$\|\delta\|_{mean}$							0.34

[1] NIST Chemistry Webbook.

For example:

1. Cubane (C_8H_8) is a set of 6 four-membered cycles ($n_{cycle} = 12 - 8 + 2 = 6$). Then

$$\Delta_c H^{gross}(C_8H_8,cr.) = 8\Delta_c H^{gross}(C) + 8\Delta_c H^{gross}(H) + 6E_4^{**} = -4815.3 \text{ kJ·mol}^{-1}, \quad (13)$$

which is 17.97 kJ·mol^{-1} (~0.4%) less than the experimental value (NIST value) for the crystal.

2. The C_{60} fullerene structure consists of 12 five-membered and 20 benzene rings (see below). Thus,

$$\Delta_c H^{gross}(C_{60},cr.) = 60\Delta_c H^{gross}(C) + 12E_5^{**} + 20E_{benz.}^{**} = -25277 \text{ kJ·mol}^{-1}, \quad (14)$$

which differs by about 2.8 % from the experimental value of the enthalpy of combustion for C_{60} fullerite = −25956 kJ·mol^{-1} [19]. Naturally, cage strain energy should be an individual characteristic of hydrocarbons such as tetrahedranes, prismanes, and icosahedranes [20], but the cage strain will most likely not exceed ~1% of the $\Delta_c H^{gross}(C_nH_m,cond.)$ kJ·mol^{-1} value.

Benzene derivatives are a special group of hydrocarbons. Conjugation effects increase the energy stability of liquid benzene. This is accompanied by a decrease in the molecule geometrical dimensions and an increase in the liquid density. Thus, *n*-hexane, cyclohexane, benzene have densities of 0.655, 0.7785, and 0.8790 g·cm^{-3}, respectively [7]. According to our estimations, the mean value of the stabilization energy of the phenyl fragment is 35.37 kJ·mol^{-1}. Thus, the final formula for calculating the mass (molar) energy of combustion is

$$\Delta_c H^{gross}(C_nH_m) = n\Delta_c H^{gross}(C) + m\Delta_c H^{gross}(H) + \sum n_{i,cycle}E_i^{**} + n_{benz.}E_{benz.}^{**}, \quad (15)$$

where $n_{benz.}$ is the number of benzene rings in the C_nH_m molecule.

VOLUMETRIC ENERGY INTENSITY OF C_nH_m HYDROCARBONS $\Delta_c H(C_nH_m)$ MJ·dm^{-3} (kJ·cm^{-3})

The volumetric energy intensity of hydrocarbons is also one of the most important characteristics of reactive fuels. Various theoretically substantiated procedures for calculating the densities or molecular volumes of substances in condensed phases can be used to predict it [5, 21–24]. To implement the main task of this work, it is most likely advisable to use simple additive procedures similar to those previously used for calculating mass energy intensities. The proposition about the additivity of the molecular volumes of hydrocarbons appears to be physically justified. It can be approximately represented as equation (16):

$$V_m(C_nH_m) \text{ см}^3\text{·моль}^{-1} = nV_m(C) + mV_m(H) + \sum n_{i,cycle}V_i + n_{benz.}V_{benz.}, \quad (16)$$

where $V_m(C)$ and $V_m(H)$ are the molar volumes of the C and H atoms in hydrocarbons, and V_i is the parameter that accounts for the influence of cycles (double bonds) in molecules on $V_m(C_nH_m)$.

Thus, the volumetric energy intensity of hydrocarbons can be calculated using equations (17) or (18):

$$\frac{\Delta_c H^{gross,net}(C_nH_m) \text{ kJ·mol}^{-1}}{V_m(C_nH_m) \text{ cm}^3\text{·mol}^{-1}} = \Delta_c H^{gross,net}(C_nH_m) \text{ kJ·cm}^{-3}, \quad (17)$$

$$\frac{n\Delta_c H(C) + m\Delta_c H(H) + \sum n_{i,cycle}E_i^{**} + n_{benz.}E_{benz.}^{**}}{nV_m(C) + mV_m(H) + \sum n_{i,cycle}V_i + n_{benz.}V_{benz.}} = \Delta_c H(C_nH_m) \text{ kJ·cm}^{-3}. \quad (18)$$

The additive constants of molecular volumes for 75 liquid C_nH_m hydrocarbons with n = 6–16 and different molecular structures were calculated using the d^{20} values (g·cm^{-3}) found in the data from [7]. The $V_m(C)$, $V_m(H)$ and V_i values (Table 7) were obtained in the first version of calculations using the least squares method. They reproduced the experimental values with a mean absolute error of $|\delta|_{mean}$ = 0.89%. However, it is difficult to explain the physical meaning of the obtained constants, particularly $V_m(C)$ = −16.618 cm^3·mol^{-1}.

In the second version of the calculation, we used the value of the hydrogen atom volume, $V(H) = (2.0 \times 10^{-8})^3$ cm^3, obtained by Askadskii and Matveev [21]. This value corresponds to $V_m^{'}(H)$ = 1.205 cm^3·mol^{-1}. If we assume that the packing density of molecular liquids is $K \approx 0.6$, then $V_m(H) \approx 2.0$ cm^3·mol^{-1}. Table 7 shows other $V_m(C)$ and V_i values that reproduce the values of $V_m(C_nH_m)$ with a relative mean deviation of $|\delta|_{mean}$ = 3.79%. As a cycle forms due to the loss of two H atoms, the molar volume decreases by about $-2V_m(H) = 4$ cm^3·mol^{-1} for each cycle.

For the monocyclic C_nH_{2n} hydrocarbons, the larger the cycle size at i = 2–6, the larger the decrease in the molecular volume, and accordingly, the increase in the density since $V_2 > V_3 > V_4 > V_5 > V_6$.

Figure 2 is a comparison of the densities (d, g·cm^{-3}) of C_nH_m hydrocarbons at n = 6. As shown in the figure, the loss of each pair of hydrogen atoms increases the density of the hydrocarbons.

Table 7. Additive constants for calculating molecular volumes $V_m(C_nH_m)$

V_m, cm^3·mol^{-1}	V_m(C)	V_m(H)	V_2	V_3	V_4	V_5	V_6	$V_{benz.}$	$\|\delta\|_{mean}$
I	−16.62	16.41	24.74	22.89	20.00	15.17	12.08	91.90	0.89
II	15.34	2.0	1.7	−0.13	−1.65	−11.42	−26.06	−26.57	3.79

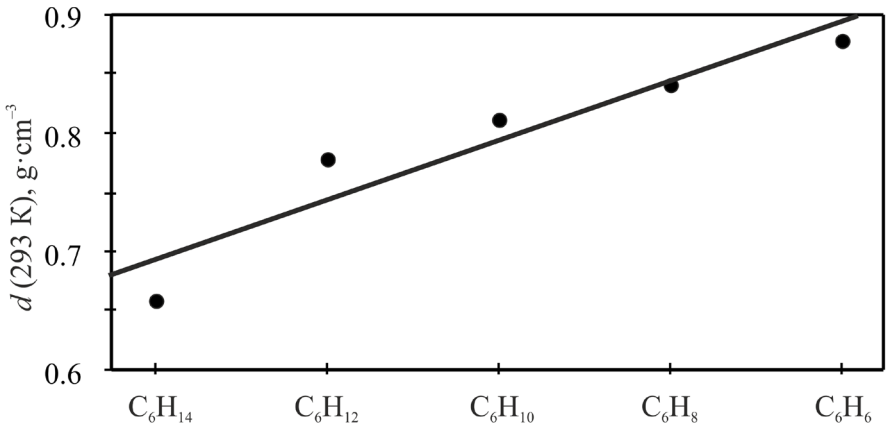


Fig. 2. Dependence of the density of hydrocarbons (hexane, cyclohexane, cyclohexene, 1,3-cyclohexadiene, and benzene) on the composition at n = 6 according to [7].

Thus, simultaneously achieving the maximum values of the mass and volumetric energy intensities of hydrocarbons appears improbable, and the optimization procedure is difficult. C_nH_m hydrocarbons with high m/n values and 4,5,6-membered rings in their molecular structures may have relatively high mass and volumetric energy intensities simultaneously.

The volumetric energy intensity of fuels with high mass energy intensity can be increased by adding high-density carbon substances to them. We have demonstrated [25] that using nanotubes significantly increases the volumetric energy intensity of hydrocarbon fuels.

CONCLUSIONS

The above analysis of the molar and mass enthalpy of combustion (energy intensity) of C_nH_m hydrocarbons suggests that the following statements are true:

1. The m/n ratio, not the presence of a large number of small carbon cycles in the molecules, is the decisive factor for achieving high values of molar and mass energy intensity of C_nH_m hydrocarbons (kJ·mol^{-1}, MJ·kg^{-1}).

2. As the cycles in C_nH_m molecules occur, the number of hydrogen atoms by two atoms per cycle. This results in a decrease of $2\Delta_cH^{gross}(H) = -223.38$ kJ·mol^{-1} in the energy intensity, and in condensed hydrocarbons, this decrease is not compensated by the arising strain energy.

3. The highest mass energy intensity is found in n-alkanes, which are extracted from oil fractions using well-developed technology.

4. For quick estimates of the values of the molar and mass energy intensity of hydrocarbons at 298.15 K with an error of about 1%, it is logical to use simple relations:

$$\Delta_cH^{net,gross}(C_nH_m)_{liq.,cr.} = \left[n\Delta_cH^{net,gross}(C) + m\Delta_cH^{net,gross}(H)\right], \text{kJ}\cdot\text{mol}^{-1}$$

$$\Delta_cH^{net,gross}(C_nH_m)_{liq.,cr.} = \left[m_C\Delta_cH^{net,gross}(C) + m_H\Delta_cH^{net,gross}(H)\right], \text{MJ}\cdot\text{kg}^{-1}$$

5. Owing to the unique nature of these properties, a separate analysis is required to justify the method for predicting molar volumes (V_m (dm^3·mol^{-1})), densities (d (kg·dm^{-3})), and volumetric combustion energies (MJ·dm^{-3}).

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Authors' contribution

G.J. Кабо – developing the scientific work concept, writing the text of the article;

L.A. Kabo – collecting and processing the material, making calculations;

L.S. Karpushenkava – making calculations, writing the text of the article;

A.V. Blokhin – writing the text of the article, offering consultations on methodology and research.

The authors declare no conflicts of interest.

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About the authors:

Gennady J. Kabo, Dr. Sci. (Chem.), Professor, Professor of the Department of Physical Chemistry, Belarusian State University (14, Leningradskaya ul., Minsk, 220030, Belarus). E-mail: kabo@bsu.by. Scopus Author ID 56261611100

Lubov A. Kabo, Student, Department of Functional Analysis and Analytical Economics, Belarusian State University (4, Nezavisimosti pr., Minsk, 220030, Belarus). E-mail: alvykabo@gmail.com. https://orcid.org/0000-0003-2620-3749

Larisa S. Karpushenkava, Cand. Sci. (Chem.), Associate Professor, Associate Professor of the Department of Physical Chemistry, Belarusian State University (14, Leningradskaya ul., Minsk, 220030, Belarus). E-mail: karpushenkava@bsu.by. Scopus Author ID 6504468775, ResearcherID AAB-8934-2020, https://orcid.org/0000-0002-8875-5568

Andrey V. Blokhin, Dr. Sci. (Chem.), Professor, Head of the Department of Physical Chemistry, Belarusian State University (14, Leningradskaya ul., Minsk, 220050, Belarus). E-mail: blokhin@bsu.by. Scopus Author ID 7101971167, ResearcherID AAF-8122-2019, https://orcid.org/0000-0003-4778-5872

Об авторах:

Кабо Геннадий Яковлевич, д.х.н., профессор, профессор кафедры физической химии Белорусского государственного университета (Беларусь, 220030, Минск, ул. Ленинградская, д. 14). E-mail: kabo@bsu.by. Scopus Author ID 56261611100

Кабо Любовь Андреевна, студентка кафедры функционального анализа и аналитической экономики Белорусского государственного университета (Беларусь, 220030, Минск, пр. Независимости, 4). E-mail: alvykabo@gmail.com. https://orcid.org/0000-0003-2620-3749

Карпушенкова Лариса Степановна, к.х.н., доцент, доцент кафедры физической химии Белорусского государственного университета (Беларусь, 220030, Минск, ул. Ленинградская, д. 14). E-mail: karpushenkava@bsu.by. Scopus Author ID 6504468775, ResearcherID AAB-8934-2020, https://orcid.org/0000-0002-8875-5568

Блохин Андрей Викторович, д.х.н., профессор, заведующий кафедрой физической химии Белорусского государственного университета (Беларусь, 220030, Минск, ул. Ленинградская, д. 14). E-mail: blokhin@bsu.by. Scopus Author ID 7101971167, ResearcherID AAF-8122-2019, https://orcid.org/0000-0003-4778-5872

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