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# SAFETY OF TECHNOLOGICAL PROCESSES AND PRODUCTION

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## THE IMPACT OF THE STRUCTURE OF LINEAR HYDROCARBONS ON THE AUTO-IGNITION TEMPERATURE

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*Abstract.* Using experimental data available in the literature the auto-ignition temperature of saturated and unsaturated hydrocarbons with different molecular structures is analyzed. Based on modern research of hydrocarbons oxidation with different structures at high temperatures, the connection between chemical structure, bond strength in the molecule and radical mechanisms of oxidation processes with the auto-ignition temperature is shown. It is noted that the branching of molecules contributes to the temperature of self-ignition increase, that is, an increase in their composition of methyl groups, tertiary and quaternary carbon atoms located nearby in the carbon chain. Double and triple bonds, starting from C<sub>5</sub>, strengthen the molecule. The elongation of both the main chain and the chain of substituents reduces the auto-ignition temperature of the compound.

*Keywords:* linear saturated and unsaturated hydrocarbons, auto-ignition temperature, fire hazard

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### Introduction

Hydrocarbons, that is, compounds containing only carbon atoms and hydrogen are the most common organic low-molecular natural compounds. Natural fuels (gas and oil) consist of hydrocarbons; they are widely used in industry as sources of thermal energy, raw materials for organic synthesis, and solvents. All hydrocarbon compounds have a combustibility coefficient greater than one, that is, they are substances that pose a significant fire hazard. Moreover, this danger remains at all stages of production, transportation, processing and use of these compounds. The ability of a substance to spontaneously ignite creates a potential fire hazard wherever flammable materials are handled. The auto-ignition temperature is used as an important input parameter for determining the possible consequences of a leak of flammable liquids, establishing safe temperatures during industrial operation and laboratory equipment, when optimizing the operation of diesel and internal combustion engines.

An increasing number of organic compounds are used in industry and scientific laboratories, the variety of technological processes with their participation is growing, but the number of substances studied lags behind the number of known and used ones. The objective of the study is not only to determine the physicochemical properties of hydrocarbons, but also to characterize their fire and explosion hazard. Experimental determination of the properties of each substance is not always advisable or practically impossible. The development of methods that can replace experimental ones and make it possible to predict the required values of properties had been extremely relevant in scientific research community and was called Quantitative Structure-Property Relationship (QSPR) [1].

A huge impetus for the development of QSPR methods was given by the emergence of computer technologies that make it possible to process large amounts of data and derive regression dependencies for calculating indicators based on the composition and structure of a compound, that is, its structural groups and physicochemical parameters.

In the Russian Federation, Federal law № 123-FZ «Technical regulations on fire safety requirements» and GOST 12.044–89 «Fire and explosion hazard of substances and materials, Nomenclature of indicators and methods for their determination» are in force; they include more than twenty indicators of fire and explosion hazard. The international safety data sheets MSDS (Material Safety Data Sheet), as a rule, provide five fire hazard characteristics: lower and upper flammability concentration limits (CFL), heat of combustion of the substance, flash point (t<sub>fsp</sub>) and auto-ignition temperature (t<sub>AIT</sub>) [1–3].

The corresponding formulas for calculating the CFL, flash points, ignition, temperature limits of flame propagation based on the boiling point and molecular structure are given in GOST, Recommendations of the VNIPO EMERCOM of Russia, reference book written by A.Ya. Korolchenko and provide good compliance between the results and the experimental values [1–6].

It is more difficult to select a method for calculating the auto-ignition temperature, since this process is associated with the oxidation of a hydrocarbon molecule with oxygen and occurs in several stages and, along with external factors and process conditions, depends on the length of the carbon chain, the strength of the carbon-carbon and carbon-hydrogen bonds on individual sections of the chain, the presence of double and triple bonds and cyclic structures and the mutual influence of atoms and groups of atoms in the molecule [7–9].

Since t<sub>AIT</sub> is the temperature at which a material spontaneously ignites upon contact with the environment, it depends not only on chemical and physical properties of the substance, but also on the methods and devices used for its determination, that is, on pressure, oxygen concentration, volume and material of the vessel etc. In different sources, especially foreign ones, the values of t<sub>AIT</sub> for the same compounds, depending on the determination method, differ up to 300 °C. To detect the sudden appearance of a flame inside the device, visual inspection is used, which introduces an error of up to 30 °C. Determining the auto-ignition temperature experimentally is very labor-intensive and not always feasible. The ability to estimate the value of t<sub>AIT</sub> using mathematical modeling eliminates the disadvantages of experimental methods and makes the process economically feasible [9, 10].

Attempts to take into account all the factors influencing t<sub>AIT</sub>, using a significant amount of statistical data and computer technologies, led to the creation of complex mathematical dependencies—that take into account, using special coefficients, various characteristics and the contribution of a certain structural group to the auto-ignition temperature.

In the most common descriptor calculation method, the variables used are the physicochemical and fire hazard properties of the substance, indicators that take into account the presence of certain structural groups in the molecule, the number of carbon atoms and the quantum chemical characteristics of the molecules. Thus, in the Russian Federation, the most widely used method is to calculate the auto-ignition temperature using the average length of a chain of molecules and the method of group increments, described by A.Ya. Korolchenko [1, 4–6].

In the works of F. Gharagheizi, based on 1025 organic compounds, 146 structural groups were selected; using software, the authors predicted t<sub>AIT</sub> for various classes of organic compounds. Chen C.-C. et al., using structural descriptors, derived a formula for calculating the auto-ignition temperature of linear and cyclic hydrocarbons. The authors of the studies claim an average calculation error of 32 °C and an average percentage of errors of 4,9–5,4 % [1, 9, 11, 12].

Due to the importance of the indicator being determined, similar work is carried out in different countries. The disadvantage of these studies is that the authors, using statistical data and computer technology, do not explain from a chemical point of view the reasons why the value of the auto-ignition temperature changes in one way or another when the structure of a substance changes. Methods available for calculation do not provide sufficient accuracy, especially for

complex branched connections. Russian researchers point out the impossibility of deducing satisfying on the accuracy of mathematical dependencies for calculating  $t_{AIT}$  of unsaturated and cyclic hydrocarbons [13, 14].

The purpose of this work is:

- collection and processing of reference data on the auto-ignition temperature of linear hydrocarbons;
- search for patterns connecting the structure of linear hydrocarbons with their auto-ignition temperature and interpretation of these relationships on the basis of existing chemical knowledge, which will allow fire safety specialists, without the use of expensive equipment and complex mathematical calculations, using the structural formulas of hydrocarbon molecules, to predict the auto-ignition temperature of compounds.

### Research methods

The authors collected domestic and foreign data on the auto-ignition temperatures of linear hydrocarbons and the mechanisms of the process for compounds of various structures, the results obtained were processed and presented in the form of tables and graphs that allow predicting the range of auto-ignition temperatures for substances of similar structure.

### Research results

Alkanes are the main component of natural and artificial fuels. As the length of the linear unbranched molecule of n-alkanes increases, the auto-ignition temperature drops from 535 °C for methane to 205 °C for nonane, remaining at the level of 202–208 °C from C<sub>9</sub> to C<sub>17</sub>. Next, an increase in the self-ignition temperature is recorded, followed by its increase (Fig. 1) [4, 6, 15].

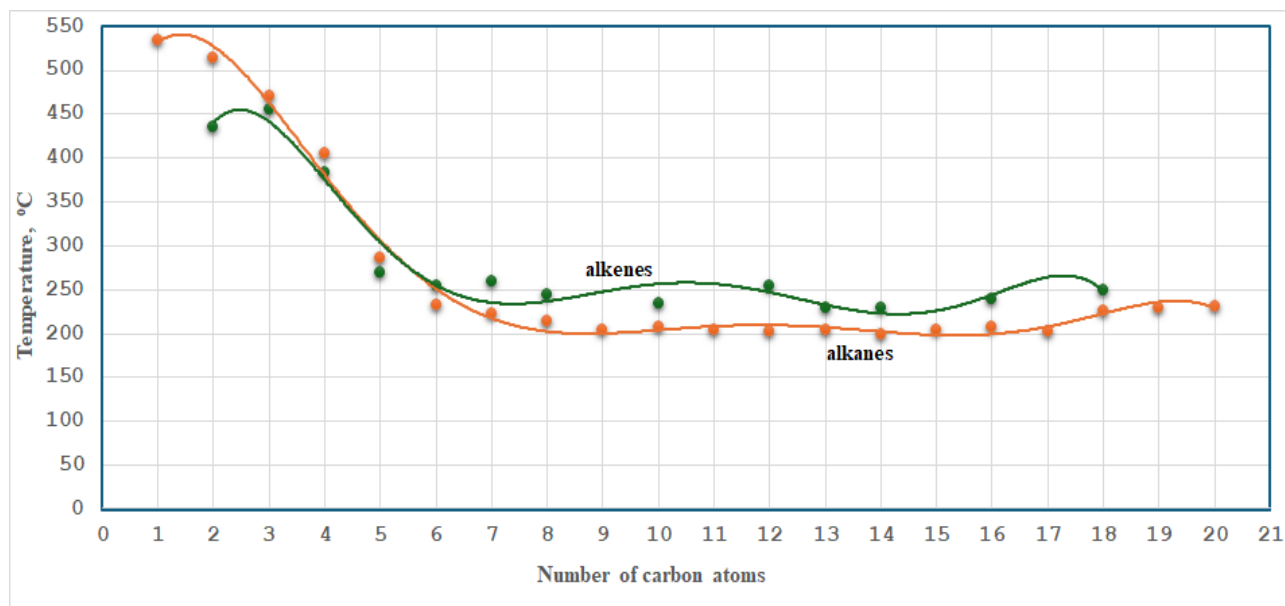


Fig. 1. Dependence of auto ignition temperatures of alkanes and alkenes-1 normal structure depending on chain length

The auto ignition temperature is an indicator of the strength of bonds in a molecule. As the length of the chain increases, internal stresses increase in it, and a significant amount of energy is spent on internal degrees of freedom: rotation and oscillation. The strength of the C–C bond decreases and, starting from the fourth–fifth carbon atom, remains constant, equal to 310,0 kJ/mol, the energy of the C–H bond also decreases (Fig. 2) [16]. The geometric configuration of the molecule changes and the ability of the fuel to react with the oxidizer is facilitated. The energy required to break these weak bonds in large molecules will probably differ slightly,

which explains the similarity of the auto-ignition temperatures of n-alkanes from nonane to heptadecane.

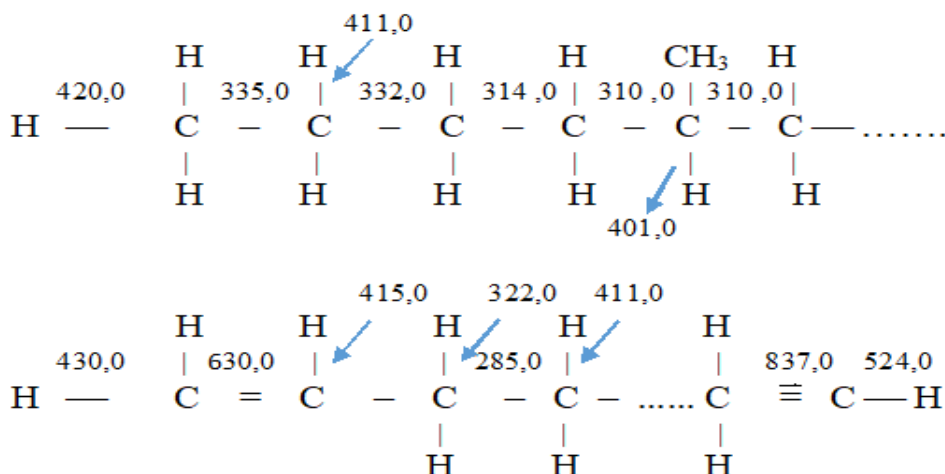


Fig. 2. Carbon-carbon and carbon-hydrogen bond energy in linear hydrocarbons molecules, kJ/mol

Isomerization does not affect the ignition limits and heat of combustion, but reduces the boiling point of organic compounds. Branched molecules are more prone to intramolecular rather than intermolecular interactions, which reduces the energy spent on evaporation and strengthens the molecule by increasing the number of methyl groups [14]. Table data 1 indicate that the self-ignition temperature decreases with increasing chain length of alkanes of similar structure (horizontal row), but increases with the appearance of substituents in the main chain, despite the general increase in the number of carbons in the molecule (vertical row).

The addition of one methyl radical increases the auto-ignition temperature, while the increase in this indicator does not depend on the position of the substituent in the chain (2-methylpentane and 3-methylpentane, 2-methylhexane and 3-methylhexane).

In molecules with short main chains ( $C_3$ – $C_4$ ), the presence of substituents has little effect; starting from  $C_5$ , the dependence of  $t_{AIT}$  on the structure of the molecule becomes more and more pronounced, so compounds with two methyl radicals are more resistant if both substituents are located on the same carbon atom, since when this creates quaternary carbon atom incapable of attaching oxygen (2,2-dimethylpentane and 2,3- or 2,4-dimethylpentane).

Presence of three and four methyl groups attached to the main chain with the formation of quaternary carbon atoms, leads to a further increase in the auto-ignition temperature, for example, for compounds 2,2,3-, 2,3,3-trimethylpentane and 2,2,3,3-, 2,2,3,4-, 2,3,3,4-tetramethylpentane has an auto-ignition temperature of 430–435 °C, which is 215–230 °C higher than that of their linear isomers n-octane and n-nonane.

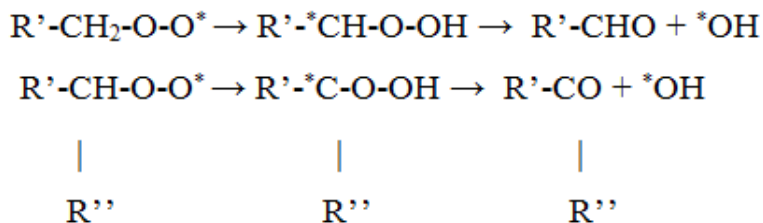
The highest self-ignition temperature is recorded if the substituents are located on neighboring carbon atoms. The appearance of  $-CH_2-$  groups between substituted carbons, especially when the main chain increases, leads to a decrease of the molecule resistance. Thus, the auto ignition temperatures of 2,3-dimethylpentane and 2,4-dimethylpentane are close (332 °C and 340 °C), and for 2,3-dimethylhexane and 2,4-dimethylhexane they already differ by 30 °C (350 °C and 320 °C),  $t_{AIT}$  of 2,2,5-trimethylhexane 330 °C, which is 50 °C lower than one's 2,3,3-trimethylhexane.

Increasing the chain length of substituents naturally reduces the auto-ignition temperature (2,4-dimethylhexane – 320 °C, 2-methyl-4-ethylhexane – 280 °C).

## Auto ignition temperatures of alkanes

Main chain, $t_{AIT}$					
C <sub>3</sub>	C <sub>4</sub>	C <sub>5</sub>	C <sub>6</sub>	C <sub>7</sub>	C <sub>8</sub>
Propane, 440 °C	Butane, 405 °C	Pentane, 286 °C	Hexane, 233 °C	Heptane, 223 °C	Oktane, 219 °C
2-methylpropane, 460 °C	2-methylbutane, 430 °C	2-methylpentane, 305 °C	2-methylhexane, 290 °C	2-methylheptane, 240 °C	2-methyloktane, 220 °C
–	–	3-methylpentane, 300 °C	3-methylhexane, 280 °C	–	4-methyloktane, 225 °C
2,2-dimethylpropane, 450 °C	2,2-dimethylbutane, 425 °C	2,2-dimethylpentane, 407 °C	–	3,3-dimethylheptane, 325 °C; 4,4-dimethylheptane, 287 °C	–
–	2,3-dimethylbutane, 435 °C	2,3-dimethylpentane, 332 °C	2,3-dimethylhexane, 350 °C	–	2,3-dimethyloktane, 225 °C; 4,5-dimethyloktane, 290 °C
–	–	2,4-dimethylpentane, 340 °C	2,4-dimethylhexane, 320 °C	2,5-dimethylheptane, 244 °C	–
–	–	2-methyl-3-ethylpentane, 350 °C; 3,3-diethylpentane, 290 °C	2-methyl-4-ethylhexane, 280 °C; 3-methyl-4-ethylhexane, 266 °C	–	–
–	2,2,3-trimethylbutane, 430 °C	2,2,3-trimethylpentane, 430 °C; 2,3,3-trimethylpentane, 430 °C	2,3,3-trimethylhexane, 380 °C; 3,3,4-trimethylhexane, 380 °C	–	–
–	–	2,2,4-trimethylpentane, 410 °C	2,2,5-trimethylhexane, 330 °C	2,5,5-trimethylheptane, 275 °C	–
–	–	2,4-dimethyl-3-ethylpentane, 390 °C	2,3,4-trimethylhexane, 360 °C	–	–
–	–	2,2,3,3-tetramethylpentane, 430 °C; 2,2,3,4-tetramethylpentane, 435 °C; 2,3,3,4-tetramethylpentane, 430 °C	–	2,2,3,3-tetramethylheptane, 360 °C	–

The oxidation mechanism of alkane self-ignition has been studied in detail and, despite its complexity and multi-stage nature, allows us to highlight some points related to with the structural features of molecules. It is assumed that the addition of oxygen occurs with the formation of peroxide and then hydro peroxide radicals, which isomerize at temperatures above 400 °C and, decomposing, turn into an aldehyde if a secondary carbon atom was oxidized, or a ketone if oxidation took place by tertiary atom [2, 8]:



The C–H bond at the tertiary atom is weaker (Fig. 2), but as a result, ketones are formed that are more resistant to further oxidation [7, 15]. (The auto ignition temperature of 2,2,5-trimethylhexane, which has two –CH<sub>2</sub>– groups in the middle of the molecule, is 330 °C, and 2,3,4-trimethylhexane, which has one –CH<sub>2</sub>– group, is 360 °C).

Having studied the spontaneous combustion of alkanes, N. Milovanovic and R. Chen found that at low temperatures, the rate of chain branching for straight-chain paraffin's is much higher than for branched ones. This is due to the structure of the \*C<sub>7</sub>H<sub>15</sub> radical, which promotes isomerization of the RO<sub>2</sub> compound and causes chain branching by ketohydroperoxide decomposition. The lower reactivity of a branched-chain alkane is due not only to the large number of less reactive methyl groups, but also to the presence of tertiary and quaternary C atoms in its structure. Hemolysis reactions of tertiary and quaternary structures compete with the formation of ketohydroperoxide, contributing to a decrease in the reactivity of branched chain paraffins. As a result, alkanes, which have a long chain and weakly bonded hydrogen atoms, have high isomerization rates and low auto-ignition temperatures, in contrast to compact and highly branched compounds with a large fraction of strongly bound H atoms, where self-ignition is inhibited [17].

Thus, it is the methylene groups that are the «weak link» in the chain. It is no coincidence that in the auto-ignition temperature group increment calculating method proposed by A.Ya. Korolchenko, the coefficient characterizing the contribution of this structure has the sign «←→» [4].

Alkenes, alkadienes and alkynes are widely used in organic synthesis, on their basis, polymerization polymers are produced, in particular rubbers. Alkenes are substances used to increase the octane number of gasoline. Alkenes formed by the processing of crude oil into gasoline by cracking heavier fractions are present in transport fuels, including gasoline, in significant quantities (up to 15–20 %). The C=C double bond is a very common functional group in biodiesel components. Alkenes serve as potential fuels or propellants for new propulsion systems. For example, jet engines that reach hypersonic speeds can be fueled with ethylene. Compounds with double and triple bonds are the main intermediate products of the alkane oxidation by spontaneous combustion processes.

The mechanism of self-ignition of unsaturated compounds has not been studied enough and, mainly, by foreign scientists [7, 18, 19]. Strength of double and triple bonds, and the carbon-hydrogen bonds at these structures is significantly higher than in alkanes (Fig. 2). It is known that the self-ignition temperature of alkenes with the same number of carbon atoms, starting from C<sub>5</sub>, is higher than that of alkanes (Fig. 1). Zhou C.-W. et al. explain this by the fact that the C–C and C–H bonds at the carbon atom located in the β-position to the double bond are much weaker than in other positions (Fig. 2). As a result, H abstraction reactions leading to the formation of allylic radicals (CH<sub>2</sub>=CH–CH<sub>2</sub>–) at high temperatures in C<sub>5</sub> and higher alkenes occur more easily than the addition of a radical to the double bond, which is typical for smaller alkenes. In addition, at high temperatures, the C=C bond absorbs Ḣ and Ö̇ radicals, which reduces the reactivity of alkenes compared to paraffines [19].

Bouncer R. et al. determined that increasing the degree of substitution at the double bond and moving it inside the molecule makes the compound more stable (alkene-3 > alkene-2 > alkene-1), as a result, the octane number of isomeric alkenes increases. This is explained by the appearance of trans-isomers in alkenes-2 and alkenes-3, which are stronger compounds than cis-isomers [7, 18]. Table data 2 does not confirm the assumption that auto ignition temperature increases with the moving of double bond, this may be due to the fact that the shift of the C=C double bond

to the central part of the molecule interrupts the formation of branched chain alkenylketohydroperoxides and, therefore, reduces reactivity at low temperatures, but accelerates reactivity at high temperatures [19].

Table 2

### Auto ignition temperatures of linear unsaturated hydrocarbons

Main chain, $t_{AIT}$				
$C_3$	$C_4$	$C_5$	$C_6$	$C_7$
Propene, 455 °C	Butene-1, 384 °C; Butene-2, 324 °C	Pentene-1, 270 °C; Pentene-2, 273 °C	Hexene-1, 254 °C Hexene-2, 245 °C	Heptene-1, 260 °C
2-methyl- propene, 465 °C	2-methylbutene-1, 365 °C; 2-methylbutene-2, 380 °C	2-methylpentene-1, 300 °C; 2-methylpentene-2, 240 °C	–	–
–	3-methylbutene-1, 374 °C	4-methylpentene-1, 305 °C; 4-methylpentene-2, 330 °C	–	–
–	2-ethylbutene-1, 324 °C	–	–	–
–	2,3-dimethylbutene-1, 369 °C; 2,3-dimethylbutene-2, 400 °C	–	–	–
–	–	2,3,3-trimethyl- pentene-1, 383 °C; 2,4,4-trimethyl- pentene-1, 365 °C	–	–
–	Butadiene-1,3, 430 °C	Pentadiene-1,3, 430 °C	Hexadiene-1,5, 350 °C	–
–	2-methylbutadiene-1,3, 400 °C	–	–	–
–	Butin-1, 386 °C	Pentin-1, 281 °C	Hexin-2, 290 °C	Heptin-1, 255 °C
–	3-methylbutin-1, 263 °C	–	–	–
–	Butene-1-in-3, 310 °C	–	–	–
–	2-methylbutene-1-in-3, 260 °C	–	–	–

Just as in alkanes,  $t_{AIT}$  of olefins increases with branching. The appearance of a second double bond increases the auto ignition temperature. Replacement of a double bond with a triple bond in acetylene comparing with ethylene reduces  $t_{AIT}$  on 100 degrees. Chain length elongation causes the increasing of alkynes resistance so alkynes  $t_{AIT}$  differs little from similar alkenes; however, branching of alkynes or replacing one double bond with a triple one leads to decrease of the spontaneous ignition temperature of compounds (Table 2). Thus, it is impossible to predict the behavior of linear unsaturated compounds based only on bond strength indicators; a large amount of additional research is required on the influence of double and triple bonds on spontaneous ignition processes.

## Conclusion

Existing methods for estimating the self-ignition temperature of substances are very complex, costly, do not always take into account the structural features of molecules and the mechanism of oxidation processes, and do not provide the required accuracy. Availability of isomers or homologues data close in structure to the substance under study, characteristics their self-ignition chemical behavior makes it possible to predict the indicator and evaluate the obtained calculated values. When predicting the fire hazard of linear hydrocarbons, it should be taken into account that the self-ignition temperature increase is contributed by the branching of molecules, an increase in the number of methyl groups and double bonds. The molecule auto-ignition resistance is higher, the more tertiary and quaternary carbon atoms it contains and the closer the substituents are located in the molecule. Double and triple bonds, starting from C<sub>5</sub>, strengthen the molecule. Elongation of both the main chain and the substituent chain reduces the auto ignition temperature of the compound.

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