r([Py–]N…H[–CX_3] was also estimated and closely related to the magnitude of ν_1. Moreover, the molecular orbitals of hydrogen bonding complex from HOMO-4 to HOMO were analyzed to explain their roles in the ring vibrations of pyridine. The triangle vibration turns to be much less sensitive to the pyridine involved hydrogen bonding. The sequence in the magnitude of ring breathing vibration frequency blue shift for haloforms is against the sequence of the electronegativity of halogen atoms because the hydrogen bond formation involves the redistribution of both σ and π electrons, as well as the halogen atoms in haloforms acting as electron lone pair donors in [Py–]H…X[–CHX_2] hydrogen bond.

STUDYING OF CETANE-INCREASING ADDITIVES EFFECT ON THE QUALITY OF DIESEL FUEL

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Diesel fuel is one of the most demanded fuel for automobiles [1]. Each customer, depending on the region, chooses the most different additives to fuels, and they, in turn, are regulated both by the accuracy of the dosage and by quantity entering into fuel. In this regard, the plants are made directly to the needs and needs of the customer, in order to qualitatively realize the compounding of fuel.

In the production of diesel fuels, it is necessary to add certain additives to improve its characteristics and achieve the required quality. There are the following types of additives: depressant, cetane-boosting, anti-wear, depressant-dispersant, lubricating, antistatic, antioxidant.

Cetane-boosting additives are designed to improve the inflammability of diesel fuels in the combustion chamber. In domestic practice, they are used very rarely, since the proportion of straight-run diesel fractions with a high cetane number (TCH) is high in the fuel balance of the country. Highly aromatic middle distillate fractions of various origins

Table 1. Process conditions

Temperature, K	Pressure, atm	Distance between molecules, Å
298	1	4

Table 2. Energy of interaction of the additive with isoparaffins

Component of diesel fuel	E, kkal/mole	E, kJ/mole • K'
Isopropylnitrate	73.74	308.54
3-ethyldecane	238.83	999.29
isopropylnitrate + 3-ethyldecane	328.20	1373.20
Δ	15.61	65.34
2,2,4,4,6-pentamethylheptane	237.40	993.30
isopropylnitrate + 2,2,4,4,6-pentamethylheptane	327.24	1369.18
Δ	16.09	67.32
2,5-dimethylundecane	257.28	1076.45
isopropylnitrate + dimethylundecane	347.09	1452.22
Δ	16.06	67.22
5-buthylnonnan	257.67	1078.12
isopropylnitrate + 5- buthylnonnan	347.32	1453.20
Δ	15.90	66.52
4,5-diethyloctane	238.11	996.27
isopropylnitrate + 4,5- diethyloctane	328.06	1372.60
Δ	16.20	67.78

are characterized by poor flammability. Additives are added to diesel fuels from naphthenic base oils, as well as to fuels from gas condensates, distributed in oil production sites [2].

In this paper, the effect of a cetane-increasing additive on such parameters of diesel fuel as Free Energies, Enthalpies, Entropies, heat capacity and total energy is considered.

In this work using quatum-chemical methods the influence of hydrocarbons of diesel range and cetane improving additive was studied thought such parameters as Gibbs free energy, enthalpy, entropy

Calculations on the effect of the additive on the parameters of diesel fuel were carried out using the software product Gaussian. As an additive, isopropyl nitrate was used. The process conditions are shown in Table 1. The results of the calculations in Table 2.

Since the value of the energy of isopropyl nitrate interaction with the studied isoparaffins under standard conditions was positive, it indicates the presence of an energy barrier for the formation of intermolecular bonds between these molecules of compounds of 65–67 kJ. That testifies, on the one hand, about possible other mechanism (radical) of interaction of isopropyl nitrate with isoparaffins, and on the other – about possible need of change of thermobaric conditions (temperature, pressure) for increase of reception of isopropyl nitrate to isoparaffins in diesel fuels that will become a subject of further researches.

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USING COMPUTER MODELING SYSTEM TO STUDY THE INFLUENCE OF PRESSURE ON THE PROCESS OF CATALYTIC DEWAXING

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The process of catalytic dewaxing is aimed to produce diesel fuel, having low freezing temperature from –18 °C to –60 °C. The fuel in this case is called winter diesel fuel and arctic diesel fuel [1].

The freezing temperature is mainly determined by the content of long straight-chain paraffins [2]. These normal paraffins undergo the reaction hydrocracking in the process of catalytic dewaxing to form short-chain normal paraffins and iso-paraffins, which have much lower freezing points [3].

The aim of this work is to study the influence of pressure on the process of catalytic dewaxing.

To perform calculations, computer modeling system of the catalytic dewaxing process was applied. This system is based on the mathematical model of the process.

As the initial data, two different feedstock compositions were used. The feedstock differs by the content of long-chain normal paraffins. The content of n-paraffins in the first feedstock is 14 wt.%. The content of n-paraffins in the second feedstock is 21 wt.%. For each of these feedstock compositions the study of pressure influence on the process of catalytic dewaxing was studied. Technological parameters for the calculations were taken as: feedstock flow rate was 280 m^3/h, flow rate of hydrogen-containing gas was 20000 m^3/h, temperature was 340 °C.

As a result, the following relations were obtained:

1. Relation between the pressure and the content of n-paraffins C_{10}–C_{27} in the product for the first (fig. 1a) and the second (fig. 1b) composition.
2. Relation between the pressure and the cold filter plugging point of the product for the first (fig. 2a) and the second (fig. 2b) composition.
3. Relation between the pressure and the yield of the product for the first (fig. 3a) and the second (fig. 3b) composition.