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Nanostructured Energy Characteristics of Hydrocarbon Hydrogen Containing Fuels

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Abstract

The consistent calculations of bond energy in cluster water nanostructures have been performed following the P-parameter methodology and quantum-mechanical methods. The formation of high energy bonds in the process of hydrocarbon hydrogen containing fuel preparation has been explained.

Keywords: Spatial-energy parameter; Cluster water nanostructures; High energy bonds

Introduction

Water plays the ambiguous role in hydrocarbon fuel of internal combustion engines. On the one hand, simple dilution of petroleum or diesel fuel with water can significantly deteriorate technological characteristics of the fuel. As soon as water drops get into cylinders, the following happens: in the compression stroke when both valves are closed, the piston bears against the water plug when moving upwards. The pressure inside the cylinder increases multiply. The engine tries to bring the connecting rod to the upper position, continuing the cycle. In fact, the pistons in one or several cylinders stop at once, and the crankshaft which continues rotating takes enormous loads. It bends connecting rods, breaks piston pins and often breaks down itself. On the other hand, optimal water content in hydrocarbon fuel is defined by the standard technological norm of such fuel mixture which is prepared by a special technique. Moreover, based on the invention patent [1] water containing fuel can have the potential energy of 1/3 from energy unit of ВТИ - petroleum, and nevertheless the engines produce the same power as with additional amount of petroleum by the mass equaled to the mass of water added. And you not only have the power gain, but you also benefit in fuel technological characteristics, such as fire safety, octane number, application temperature limits, possibility to use cheaper fuels, etc. Such specificity of technological processes is ultimately defined by the mechanism of physic-chemical transformations occurring on atom-molecular level. In this investigation their possible evaluations are studied based on the concept of spatial-energy parameter (P-parameter).

Formation of high energy bonds in fuel mixture

Practical use of hydrogen containing fuel is possible only if a number of conditions are fulfilled:

1. Introduction of complex additives into the fuel, with alcohols and so-called “hydrogen catalyst” content having the primary meaning.
2. Such additives are mixed following the special technique - first, by separate fractions, and in the end all the mixture is intensively stirred by a hydraulic cutting pump (hydraulic shears).

According to the author [1], “hydrogen catalyst” contributes to active dissociation of water molecules with the formation of hydrogen and oxygen which burn in the engine chamber afterwards. But is not clear how during such a short combustion time of the given amount of mixture introduced into the chamber, water dissociation in this volume and burning of its products can take place. Moreover, as a result of water dissociation by the reaction $H_2O=H^++OH^-$ the direct oxygen release is not observed. Obviously, other important mechanisms of physic-chemical transformation of energy are involved. For instance, it is known that as a result of biochemical reactions in the presence of certain ferments the synthesis of ATP molecule can take place whose potential energy increases due to the formation of special high energy bonds.

It is possible that similar processes take place during the formation of burning mixture of this type of fuel when nanoclusters in the form of fullerenes can be formed under certain technological conditions. First of all, this is aided by the introduction of alcohols into the fuel mixture that results in the formation of fullerene, for example, $C_{60}(OH)_{10}$. Therefore, the addition of alcohols (up to 20%) just corresponds to the ratio of molar masses of hydroxyl groups OH^- and carbon atoms. At the second stage of fuel preparation, high energy bonds are formed in the systems $C_{60}(OH^-)$-n(H_2O), first of all, due to the introduction of "hydrogen catalyst" into the mixture, and besides, when filtering water through the coal filter which contributes to the extraction of nanostructured formations of carbon atoms into the mixture.

Similar to ATP hydrolysis which is accompanied by the release of chemical bond energy, the breakage of high energy bonds and heat energy release occur in hydrogen containing fuel when it is burning in the engine chamber. The physic-chemical mechanism of the formation of energy saturated bonds in this system is given below.

Investigation technique

The value of the relative difference of P-parameters of interacting atom-components-coefficient of structural interaction α was used as the main numerical characteristic of structural interactions in condensed media [2]:

$$\alpha = \frac{\text{Đ}_1 - \text{Đ}_2}{(\text{Đ}_1 + \text{Đ}_2)/2} 100\% \quad (1)$$

Applying the reliable experimental data, we obtain the nomogram of the dependence degree of structural interactions upon coefficient α -unified for the wide range of structures (no Figure is available). This approach allows evaluating the degree and directedness of structural interactions of phase formation, isomorphism and solubility processes in multiple systems, including molecular ones. In particular, the features of cluster formation in the system $CaSO_4$-H_2O have been investigated [3].

To evaluate the directedness and degree of phase formation processes [1] the following equations are used:

1. Initial values of P-parameters:

$$\frac{1}{q^2/r_i} + \frac{1}{W_i n_i} = \frac{1}{P_{\mathring{A}}}; \quad \frac{1}{P_0} = \frac{1}{q^2} + \frac{1}{(Wrn)_i}; \quad P_{\mathring{A}} = P_0/r_i; \quad (2, 3, 4)$$

here: W_i-electron orbital energy [4]; r_i-orbital radius of *i* orbital [5]; $q = Z^*/n^*$-by [6,7]; ni-number of electrons of the given orbital, Z^* and n^*-effective nucleus charge and effective main quantum number. P_0 is called as spatial-energy parameter, and P_E-effective P-parameter.

Table 1: P-parameters of atoms calculated via the electron bond energy.

Atom	Valence Electrons	W (eV)	r_i (Å)	q^2 (eV Å)	P_0(eV Å)	R (Å)	$P_E=P_0/R$ (eV)
H	$1S^1$	13.595	0.5295	14.394	4.7985	0.5295	9.0624
H	$1S^1$					0.28	17.137
C	$2P^1$	11.792	0.596	35.395	5.8680	0.77	7.6208
C	$2P^1$					0.69	8.5043
C	$2P^2$	11.792	0.596	35.395	10.061	0.77	13.066
C	$2S^1$	19.201	0.620	37.240	9.0209	0.77	11.715
C	$2S^2$				14.524	0.77	18.862
C	$2S^2+2P^2$				24.585	0.77	31.929
C	$1/2(2S^2+2P^2)$						15.964
O	$2P^1$	17.195	0.4135	71.383	4.663	0.66	9.7979
O	$2P^2$	17.195	0.4135	71.383	11.858	0.66	17.967
O	$2P^2$					0.59	20.048
O	$2P^4$	17.195	0.4135	71.383	20.338	0.66	30.815

The calculation results by equations [2-4] for a number of elements are given in Table 1, from which it is seen that for hydrogen atom the values of P_E-parameters substantially differ at the distance of orbital (r_i) and covalent (R) radii. The hybridization of valence orbitals of carbon atom is evaluated as the averaged value of P-parameters of $2S^2$ and $2P^2$- orbitals.

2. Values of P_c-parameter in binary and complex structures:

$$\frac{1}{P_{\tilde{n}}} = \frac{1}{N_1P_1} + \frac{1}{N_2P_2} + \ldots\ldots \quad (5)$$

where N-number of homogeneous atoms in each subsystem.

The results of such calculations for some systems are given in Table 2.

Table 2: Structural Pc-parameters.

Radicals, Molecules	P_1 (eV)	P_2 (eV)	P_3 (eV)	P_4 (eV)	P_c (eV)	Orbitals of Oxygen Atom
OH	17.967	17.137			8.7712	$2P^2$
OH	9.7979	9.0624			4.7080	$2P^1$
H_2O	2 × 17.138	17.967			11.788	$2P^2$
H_2O	2 × 9.0624	17.967			9.0226	$2P^2$
C_2H_5OH	2 × 15.964	2 × 9.0624	9.7979	9.0624	3.7622	$2P^1$

3. Bond energy (E) in binary and more complex systems:

$$\frac{1}{E} \approx \frac{1}{P_E} = \frac{1}{P_1(N/\hat{e})_1} + \frac{1}{P_2(N/\hat{e})_2} + \ldots\ldots\ldots \quad (6)$$

Here (as applicable to cluster systems) κ_1 and κ_2 -number of subsystems forming the cluster system; N_1 and N_2-number of homogeneous clusters [7]. So, for $C_{60}(OH)_{10}$ $\kappa_1 = 60$, $\kappa_2 = 10$.

Calculations and comparisons

It was assumed that structural-stable water cluster (H_2O) can have the same static number of subsystems (κ) as the number of subsystems in the system interacting with it [8]. For example, the water cluster n $(H_2O)_{10}$ is interacting with fullerene $[C_6OH]_{10}$.

Similarly, with cluster $[C_6OH]_{10}$ the formation of cluster $[(C_2H_5OH)_6\text{-}H_2O]_{10}$ is apparently possible, which corresponds to the system $(C_2H_5OH)_{60}\text{-}(H_2O)_{10}$. The interaction of water clusters was considered as the interaction of subsystems $(H_2O)_{60}\text{-}N(H_2O)_{60}$ [9].

Based on such concepts, the bond energies in these systems are calculated by equation (6), the results are given in Table 3. To compare, the calculation data obtained by Khokhriakov NV with quantum-chemical techniques [10] are given. Both techniques produce consistent values of bond energy (in eV). Besides, the methodology of P-parameter allows explaining why the energy of cluster bonds of water molecules with fullerene $C_{60}(OH)_{10}$ 2 times exceed the bond energy between the molecules of cluster water (Table 3). In accordance with the nomogram, the phase formation of structures can take place only if the relative difference of their P-parameters (α) is under 25-30%, and the most stable structures are formed when α <6-7%.

Table 3: Calculation of bond energy - E (eV).

System	C_{60}	$(OH)_{10}$	$(H_2O)_{10}$		P_E (eV) E (eV) (calculation)	
	P_1/κ_1	P_2/κ_2	P_3/κ_3	n_3	By equation (6)	Quantum-mechanical
$C_{60}(OH)_{10}$- $N(H_2O)_{10}$	15.964/60	8.7712/10	11.788/10	1	0.174	0,176
				2	0.188	0,209
				3	0.193	0,218
				4	0.196	0,212
				5	0.197	0,204

$(H_2O)_{60}$ - $N(H_2O)_{60}$	9.0226/60	9.0226/60		n_2		
				1 2 3 4 5	0.0768 0.1020 0.1128 0.1203 0.1274	0,0863 0,1032 0,1101 0,1110 0,115
$(C_2H_5OH)_{60}$-$(H_2O)_{10}$	3.7622/60	9.0226/10			0.0586	0.0607
$(C_2H_5OH)_{10}$-$(H_2O)_{60}$	3.7622/10	9.0226/60			0.1074	$\approx$0.116

In Table 4 different values of coefficient α in systems H-C, H-OH and H-H_2O are given, which are within 0.44-7.09(%). But in the system H-C for carbon and hydrogen atoms the interactions at the distances of covalent radii have been taken into account, and for other systems-at the distance of orbital radius. The interaction in system H-C at the distances of covalent radius plays a role of fermentative action, which results in the transition of dimensional characteristics in water molecules from the orbital radius to the covalent one and formation of system $C_{60}(OH)_{10}$-$N(H_20)_{10}$ with bond energy between the main components 2 times greater than between the water molecules (high energy bonds).

Table 4: Spatial-energy interactions in the system H-R, where R= C, (OH), H2O.

System	P_1(eV)	P_2(eV)	$\alpha = \frac{\Delta Đ}{\langle Đ \rangle}100\%$	Spatial Bond Type
H-C	17.137	15.964	7.09	Covalent
H-OH	9.0624	8.7712	3.27	Orbital
H-H_2O	9.0624	9.0226	0.44	Orbital

Thus, broad capabilities of water clusters to change their spatial-energy characteristics apparently explain all the diversity of structural properties of water in its different modifications, including the formation of high energy bonds in water containing fuel for internal combustion engines.

Conclusion

1. Results of bond energy calculations in water cluster nanostructures following the P-parameter methodology agree with quantum-mechanical methods.

2. Changes which can take place in spatial-energy characteristics of water clusters explain the formation of high energy bonds in the process of hydrocarbon fuel preparation.

3. Breaking of these bonds with the release of additional amount of heat energy occurs in the combustion chamber.

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