THE GROUNDED OF FUEL INSTALLATIONS ENERGY EFFICIENCY BY PHOTOACTIVATION OF MOLECULES REAGENTS OF COMBUSTION REACTION

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The possibility of improving the fuel efficiency of plants using molecular reagents for the combustion of optical radiation. Reasonable basic parameters of optical radiation transferred molecules of oxygen, nitrogen, methane and propane in the excited state.

Irradiation, energy, frequency, burning, molecule, activation.

The main issues of the different countries economies at the present stage is to reduce the energy component in the value of industrial and agricultural products. This is due primarily to the timing of depletion of proven and probable reserves of conventional hydrocarbon energy fuels, measured in several decades [3,7]. Prolongation use of coal, oil, natural gas and nuclear fuel is important: first - to continue the time required to conduct research substantiation of fundamentally new ways of generating energy, and secondly - to increase the use of hydrocarbon resources in the chemical and food industries; thirdly - to reduce environmental impact. Activation of combustion reaction molecules reagents is, in our opinion, one of the most promising ways to improve fuel efficiency equipment [9], which will increase the use of non-renewable fossil terms of hydrocarbon fuels, indicating that the relevance and timeliness of solution of this problem.

The purpose of research - the grounded of the method of increasing the efficiency of power generating plants by using optical radiation to activate the molecules of the combustion of gaseous reactants hydrocarbon fuels in air.

State of the problem. Activation of molecules involved in chemical reactions can be carried out in various ways. These include: thermoactivation, photroactivation, ultrasonic activation, activation of the magnetic field, the activation of an electric field, the activation of fast electrons, activation radioactive particles and so on.

At the core of the process lies teploheneruvanni redox exothermic combustion reaction. Improving the efficiency of these reactions is the main issue of chemical kinetics. Efficiency of combustion reactions depends on the properties of reactants, composition, structure and internal energy of molecules and external factors.

The basic law of chemical kinetics believe Arrhenius law [10]. The main condition of chemical reactions is aktyvovanist molecules reagents. Arrhenius Law describes the possibility of chemical reactions between molecules, reagents and connects the rate constant of a chemical reaction with the activation energy (E_A):

$$k = k_0 e^{-\frac{E_A}{RT}} \quad , \tag{1}$$

where k_0 - preeksponential constant; R - gas constant, equal to 1.987 cal / deg • mole; T - the temperature in degrees Kelvin; e - base of natural logarithms.

After logarithm left and right sides of equation (1) we obtain the formula:

$$\ln k = \ln k_0 - \frac{E_A}{RT} \quad . \tag{2}$$

For ease of calculation, we will be using non-natural and decimal logarithms:

$$\lg k = \lg k_0 - \frac{E_A}{4{,}575T} \quad , \tag{3}$$

where the 1/4, 575 - koefficient of natural logarithms in decimal, multiplied by the quantity R.

The activation energy is given by:

$$E_A = (\lg k_0 - \lg k)\,4{,}575T \quad . \tag{4}$$

By formula (4) the activation energy of the molecules directly proportional to temperature.

According to our working hypothesis, to activate molecules of reagents other than heat (E_{AT}), you can also use energy from other external factors (E_{A3}). If external energy sources provide energy pulsating flow, the frequency of which corresponds to the resonant frequency of molecular reagents, we can achieve the effect of transferring them to an active state with significantly lower energy costs.

Supplemented formula (4) the effect of molecular reagents for other factors, we get:

$$E_A = E_{AT} - E_{A3} = [\lg k_0 - \lg k - 4{,}575T] - Wb \quad , \qquad (5)$$

where W - energy is derived from external sources, eV; b - coefficient of molecular reagents external energy.

Using (5) shows that the thermal activation energy can be reduced by the use of other external activation molecules.

The sources of external energy to activate molecules reagents include, for example, electromagnetic radiation or radiation flux of charged particles. In [8] describes how to obtain molecules with desired properties of chemical bonds when exposed to electromagnetic radiation and streams of charged particles. With the flow of electromagnetic and infrared laser radiation reached initialization and increase the reactivity of substances [2].

The total energy of the molecule consists of electronic, vibrational and rotational energy. Normally, electrons moving, vibration and rotation of molecules are considered independent of each other.

The energy of an isolated molecule

$$E_м \approx E_{ел} + E_{кол} + E_{об} \quad , \qquad (7)$$

where $E_{ел}$ - energy of the electrons; $E_{кол}$ - energy vibrations of nuclei; $E_{об}$ - energy due to periodic changes in the orientation of the molecule in space.

The relationship between the three main components of the energy of the molecule is determined by the mass ratio of electrons and atomic nuclei in the molecule [11]

$$E_{ел} : E_{кол} : E_{об} = 1 : \sqrt{m/M} : m/M \quad , \qquad (8)$$

where m - mass of the electron; M - mass of the nuclei of atoms in the molecule.

Formula (7 and 8) do not consider the energy of atomic nuclei in the molecule and the energy of translational motion of the center of mass of the molecule. This is due to the fact that the energy of translational motion of the center of mass is

have not quantum nature and the energy of nuclear radiation is in the form of spectral lines super-weak intensity.

Since the ratio m / M ≈ 10^{-5}-10^{-3}, then $E_{ел} >> E_{кол} >> E_{об}$.

Proved that the $E_{ел}$ ≈ 1 - 10 eV, $E_{кол}$ ≈ 10^{-2} - 10^{-1} and $E_{об}$ ≈ 10^{-5} - 10^{-3} eV. Therefore, in most cases, we identify the energy of the molecule with the energy of the electrons.

Upon receipt of molecules photon energy greater than the work function of an electron, their electrons can leave the molecule, ie the process of ionization of molecules [4].

In quantum energy is smaller than the ionization energy, but sufficient for the transfer of an electron in an excited state, the molecule or atom is activated. Light activation molecule (photoexcitation) is the inelastic collisions with molecules and quantum of light [5]. With sufficient quantum energy electromagnetic radiation electrons of the molecule moving from stationary energy levels at arousal. This incident photon energy should be sufficient to activate the molecule - a conversion of one or more electrons at the level of arousal.

Results of studies. *The grounded of using photoactivation molecules reagents combustion reaction.* Photoactivation of molecules – participants of the chemical reactions is exposed at deals on them by photons of light. Molecules are move to higher energy levels of excitement. Levels are divided into resonant excitation (singlet) and metastable (triplet) levels. In addition to differences in the magnitude of the energy resonance at different times of the metastable dissipation [6]. For resonant levels dissipation time is 10^{-10} - 10^{-8} s. Metastable levels have a dissipation of 10^{-4} - 10^{-2} s and more. Residence time of molecules reagents on resonant levels often nedostattno to undergo chemical reactions between them. Therefore, we believe that molecular reagents should translate into metastable level. The energy of light quanta should be sufficient to transfer molecules to metastable level excitation.

Photon energy Ec is calculated by the formula

$$E_c = h_0 \nu \quad , \qquad (9)$$

where h_o - Planck's constant ($6{,}626 \cdot 10^{-34}$ J · s); ν - frequency electromagnetic waves, Hz.

Possible ways of energy conversion in the molecule is shown in Fig.

Primary energy supplied to a molecule with a quantum of light energy $h\nu_1$. If the photon energy is equal to or greater than the ionization energy E_{S0I0}, the electron can leave the molecule, becoming free electrons and thus creating a positive ion. During the first act of switching molecules on resonance level R_2 consumption energy E_{S0R2}, which depends on the utilization of primary energy $h\nu_1$. Next is the dissipation of the molecule with its transition into one of the lower energy levels in several possible ways:

- on the singlet level with the release of R_1 photon energy e_{R21};

- on the stable level of S_0 with the release of energy E_{R2S0}, even E_{S0R2} (ideal dissipation);

- from R_1 to S_0 with the release of energy E_{R1S0},

- from R_1 to metastable level M_2 with the release of a photon e_{R1M2} and photon energy e_{CR1}, characterizing the photochemical reaction activated molecule to another molecule or restructuring.

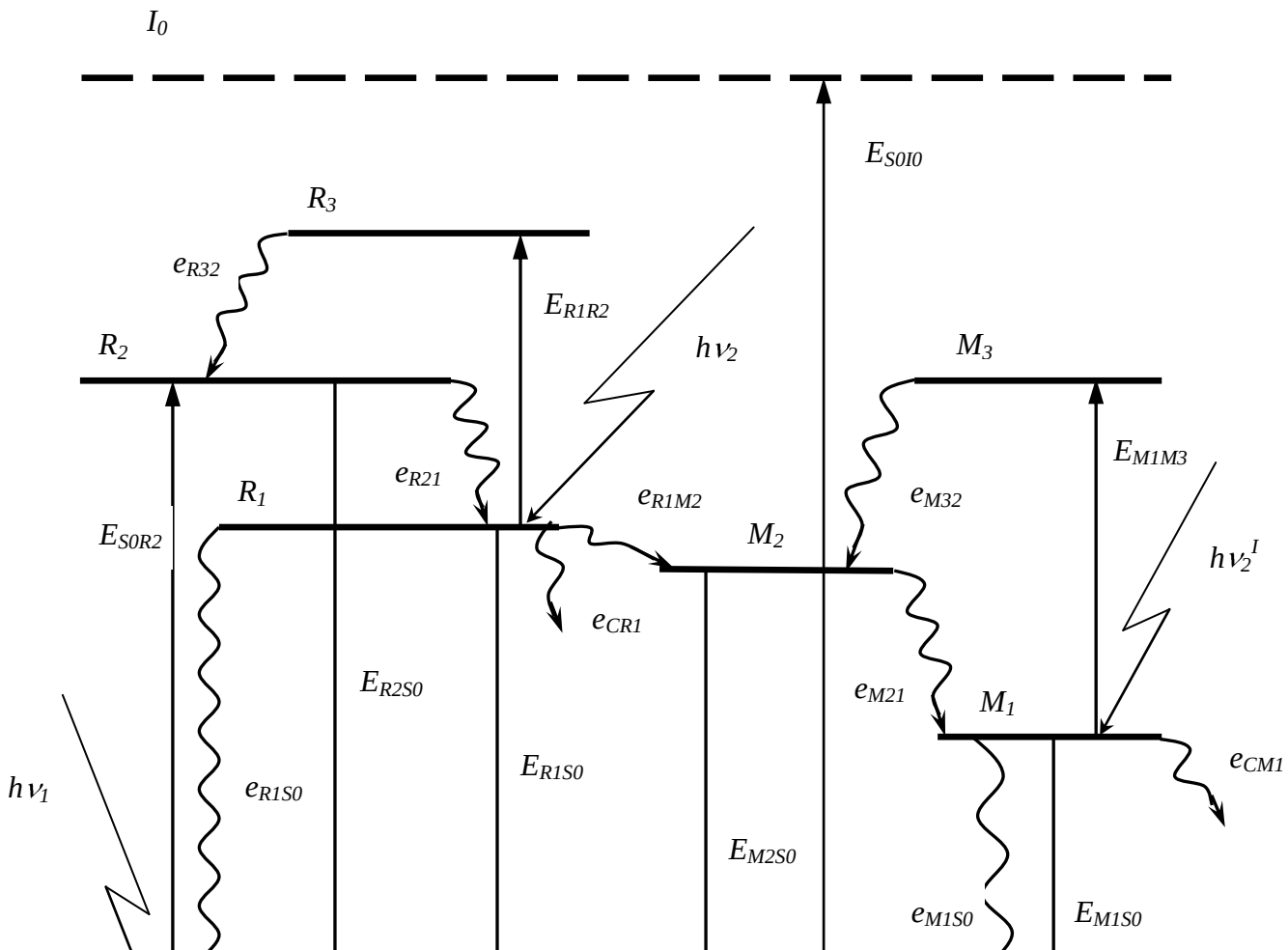

Diagram of energy levels and energy conversion in the molecule

When the energy of the molecule two or more photons ($h\nu_2$ and $h\nu_2^I$) can be achieved her transition to higher energy levels, respectively, on R_3 for energy E_{R1R3} and M_3 - E_{M1M3} energy. The transition of the molecule to a lower energy level can take place with the release of portions of energy other than optical, for example - e_{CR1} and e_{CM1}. These portions of energy can be used for photochemical reaction activated molecule with another molecule or restructuring.

Using data from [1], we calculate the frequency of electromagnetic radiation to activate the aforementioned molecules and is listed in the results table.

Options of activating electromagnetic radiation

Molecules	Energy level typ	Activation energy			Light frequency, Hz	Electro-magnetic wave lengths, nm
		eV	J/molecules	J/mol		
Methane	Singlet	11,00	$17{,}62\cdot10^{-19}$	$10{,}60\cdot10^{5}$	$2{,}65\cdot10^{15}$	113
	Triplet	9,00	$14{,}42\cdot10^{-19}$	$8{,}68\cdot10^{5}$	$2{,}17\cdot10^{15}$	138
Propane	Singlet	10,00	$16{,}02\cdot10^{-19}$	$9{,}64\cdot10^{5}$	$2{,}41\cdot10^{15}$	124
	Triplet	7,70	$12{,}34\cdot10^{-19}$	$7{,}42\cdot10^{5}$	$1{,}86\cdot10^{15}$	161
Oxygen	Singlet	9,30	$15{,}90\cdot10^{-19}$	$9{,}57\cdot10^{5}$	$2{,}24\cdot10^{15}$	134
	Triplet	4,50	$7{,}21\cdot10^{-19}$	$4{,}34\cdot10^{5}$	$1{,}08\cdot10^{15}$	278
Nitrogen	Singlet	13,00	$20{,}83\cdot10^{-19}$	$12{,}53\cdot10^{5}$	$3{,}13\cdot10^{15}$	96
	Triplet	7,35	$11{,}77\cdot10^{-19}$	$7{,}08\cdot10^{5}$	$1{,}77\cdot10^{15}$	169

As seen from the results, the transfer of molecules on the singlet level is when they are irradiated with vacuum ultraviolet radiation with a wavelength in the range from 96 nm for nitrogen to 134 nm for oxygen. Under normal conditions to obtain radiation with such parameters is problematic because of its absorption molecules closest to the source of radiation. Without special preparation of environmental parameters transfer these molecules to the singlet level not efficient.

Transfer of molecules of the combustion reactants to triplet levels can be achieved with less caution, since wavelength range, in this case, is within the 138 - 278 nm.

Conclusions

1. Efficiency of fuel equipments with gaseous hydrocarbon fuels increases in the activation of molecules reagents combustion reaction.

2. Activation of combustion reaction molecules reagents can be carried out by UV rays.

3. Transfer of molecules of methane, propane, oxygen and nitrogen in the singlet excitation level produced by irradiation with a wavelength of 96 - 134 nm.

3. Transfer of molecules of methane, propane, oxygen and nitrogen in the triplet excitation levels produced by irradiation with a wavelength of 138 - 278 nm.

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