PHYSICO-CHEMICAL SPECTRAL METHODS, MECHANISMS OF ELECTRON-NUCLEAR INTERACTIONS IN ELECTRONIC EXCITED STATES AND REACTIVITY OF SUBSTITUTED N -,O -,S-COMPOUNDS OF THE BENZENE, FURAN, THIOPHENE, OXAZOLE, OXADIAZOLE, PYRIDINE AND VARIATION OF CONDITIONS

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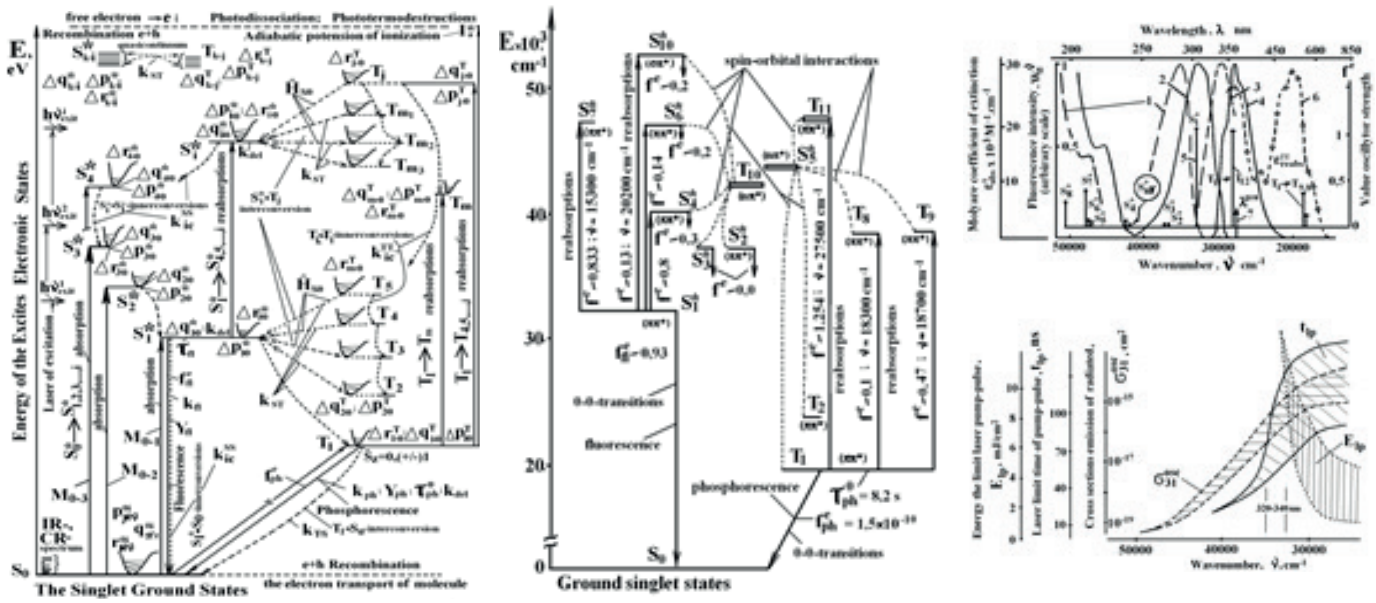
The intramolecular mechanisms of ultrafine electron-nuclear interaction forming the characteristics of the spectra: NMR, EPR, IR and UV absorption, Raman, luminescence at different temperatures (from 298 to 2,6oC) and pump types is the lasers, ions and electrons the use as additives of different functions N-,O-,S-compounds for fuel and lubricants were a studied (Fig. 1) [1].



(I) (II)

Fig. 1. (I) is the scheme of the radiative and nonradiative multistage of transitions in the full spectra S_i*T_jElExSt («elementary act») for polyatomic compounds (is doublet D*m and quartet Q*$_n$ of ions and radicals); {r_n} are the coordinates of the localized electrons on LCAO-MO-SCF-CI INDO/S for the induced of active quasioscillators in structure between the intermediate ElExSt, {l} is the quasicontinuum of inactive vibrational levels, V_n is the matrix elements of the spin-orbit interaction of factors multiplied by a Frank-Condon; V_{nl} is the matrix elements of the operator of anharmonisms, {G_n} is the width of the levels of active oscillation during of relaxation, M_{0i} is the matrix moments of electric dipole transitions. Free electron from mechanism of multistage photo-ionization. Vertical arrows is frequencies and forces the oscillators of transitions S_1*→S_0, S_1*→S_i*, T_1→S_0 and T_1→T_j formed by pumping, and $\Delta r_{\mu\nu}$, $\Delta p_{\mu\nu}$ and $\Delta q_{\mu\nu}$, $\Delta\rho_{\mu\nu}$ is the lengths, orders valence bonds, charges and total electron densities on atoms; (II) Full diagram the S_i*T_jElExSt is nπ*- and ππ*-type of the following and UV and Fluorescence spectra of the 2,5-diphenyle-1,3-oxazole (POP).

Литература
[1] Obukhov A.E. Optics and Spectroscopy, 2018, 124 (5), 696.
[2]. Obukhov A.E. Laser Physics, 1997, 7 (5), 1102.