

Electronic structure, spectral-luminescent properties and generation ability of polyatomic molecules

G.V. Mayer¹, M.V. Alfimov^{1,2}, V.G. Plotnikov^{1,2}, V.Ya. Artyukhov¹, V.A. Smirnov^{1,3}

¹Tomsk State University, 36 Lenin Ave., 634050, Tomsk, Russia, mayer_gv@tsu.ru;

²Photochemistry Center RAS, 7a Novatorov Str., 119421, Moscow, Russia;

³Institute of Problem of Chemical Physics RAS, Academician Semenov avenue 1, 142432, Chernogolovka, Moscow region, Russia

The fundamental problem of photonics of optical materials on the basis of organic compounds is to establish patterns of connection of spectral-luminescent properties and lasing ability of molecules with the features of intra- and intermolecular interactions and excitation of the electromagnetic field.

This report represents theoretical principles of molecular photonics and experimental basis of molecular photonics, discusses patterns of photophysics and photochemistry of molecular systems and their relation to electronic structure.

Application of quantum-chemical concepts and methods in the investigation of spectra and mechanisms of intramolecular photoprocesses, a theoretical estimate of the rate constant of nonradioactive (internal and intersystem) conversion, realized on the basis of semi-empirical method INDO with spectroscopic parameterization [1].

The application of molecular photonics and capabilities of spectral-luminescent systematics of molecules in the analysis of the lasing abilities of molecules are discussed. Studying photonics of organic molecules allows to conclude that only a complex (theoretical and experimental) approach to research allows to determine fundamental patterns in the mechanisms of the processes and the nature of formation of properties, gives a chance to obtain results of heuristic, predictive nature.

Mechanisms of formation and evolution of the triplet states of molecules and the formation of exciplexes in highly excited triplet states are considered.

1. Artyukhov V.Ya., Kopylova T.N., Samsonova L.G., Selivanov N.I., Plotnikov V.G., Sazhnikov V.A., Khlebunov A.A., Mayer G.V., Alfimov M.V. / A Combined Theoretical and Experimental Study on Molecular Photonics // Russ. Phys. J.– 2008.– V.51. – P. 1097–1111.