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THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE AND SPECTRAL PROPERTIES OF PHOTOACTIVE POLYMERS

I.A. Shchugoreva^{1,2,3} and F.N. Tomilin^{1,4}

¹*Siberian Federal University, 79 Svobodny Ave., 660041, Krasnoyarsk, Russia, office@sfu-kras.ru;*

²*Krasnoyarsk Science Center SB RAS, 50 Akademgorodok, 660036, Krasnoyarsk, Russia, fic@ksc.krasn.ru;*

³*Krasnoyarsk State Medical University, 1 Partizan Zheleznyak, 660022, Krasnoyarsk, Russia, rector@krasgmu.ru;*

⁴*Institute of Physics SB RAS, 50/38 Akademgorodok, 660012, Krasnoyarsk, Russia, dir@iph.krasn.ru*

In recent years, conjugated polymers have been found to be interesting materials for electronic and optoelectronic devices, such as organic light emitting diodes (OLED), transistors, and solar cells. The most important representatives of this class of polymers are 1,9-anthrazoline and 1,6-anthrazoline, because anthrazoline and its derivatives have good luminescent properties which could be tuned via variations of the type and position of substituents in the anthrazoline core. For understanding the degree of influence of various factors on the optical properties of these polymers, quantum-chemical calculations were applied.

For all the molecules, the geometry was optimized in the ground and excited states using the hybrid functional CAM-B3LYP in the 6–31G(d) basis set taking into account the solvent used, namely methanol. The absorption and luminescence spectra were calculated using the TD-DFT/B3LYP method in the cc-pVDZ basis. All the calculations were performed using the GAMESS program.

All the polymers were split into two groups: copolyamides with meta and para addition of the anthrazoline moiety. The analysis of their optical properties showed the influence of the type and position of the substituents (–CH₃, –COOH, Br–) on the spectra both of the first and second groups to be equal. The absorption and luminescence spectra of polymers from the first group are shifted to a longer wavelength region in comparison with the spectra of polymers from the second group. Their molecular orbitals would allow one to reveal the nature of this effect. First, it should be noted that for all the polymers the transition of electrons from the highest occupied molecular orbital (HOMO-1) to the lowest unoccupied molecular orbital (LUMO) orbital is responsible for the formation of absorption peaks. Electrons of the atoms from the anthrazaline fragment and carboxyl groups are mainly responsible for the formation of the LUMO orbital. However, responsible for the formation of the HOMO-1 orbital, are electrons of anthrazalin or benzene rings for the first and second group, respectively. Thus, the transition of electrons for the first group occurs within a single chromophoric group, requiring less energy than the transitions between different groups, which explains the bathochromic shift of the absorption and luminescence spectra of the first group relative to the second one.

The calculated results of these polymers will allow one to get insight into the detailed information on the structural and optical properties of the conjugated polymers. Furthermore, these results can be used for chemical modification of polymers in synthesis as well as to obtain the desired optical properties.

FLUORESCENT PROBES

O.N. Tchaikovskaya¹, V.S. Chaydonova^{1,2} and M.V. Ashmarina¹

¹*National Research Tomsk State University, 36 Lenin Ave., 634050, Tomsk, Russia;*

²*Hygienic and Epidemiological Center in Republic of Khakassia, 66 Lenin Ave., 655017, Abakan, Russia*

Fluorescence analysis methods are highly sensitive, inexpensive, easy to use, and the substances used in these methods are not toxic. Therefore, research methods related to fluorescence have been developing rather rapidly in recent decades. If a substance has its own fluorescence, its spectrum can

tell about the molecular composition of the substance without resorting to additional tools. However, most of the substances that must be investigated, have a dull fluorescence, or do not have it at all. For such cases were synthesized fluorescent probes.

The fluorescent probe binds to the molecule under investigation, and after exciting radiation transmits information about the environment in which it is located. Since the medium in which the fluorophore is located strongly affects the intensity of the fluorophore emission, the decay time of the fluorescence and the maximum of the spectrum, we can understand the composition of the solution by changing these parameters. Depending on which probe was used in the study, data on solution viscosity, temperature and polarity can be obtained.

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Y-16

INVESTIGATION OF SHG IN NEW SCANDIUM BORATE WITH THREE CATIONS BY THE KURTZ-PERRY METHOD

A.Y. Jamous¹, D.M. Ezhov¹, A.B. Kuznetsov², V.A. Svetlichnyi¹, and A.E. Kokh²

¹Tomsk State University, 36 Lenin Ave., 634050, Tomsk, Russia, ammarjamous2@gmail.com;

²Institute of Geology and Mineralogy SB RAS, 3 Koptyug Ave., 630090, Novosibirsk, Russia, ku.artemy@gmail.com

Nowadays, lasers are widely used in various technologies from medicine to space. This has created constantly growing needs to improve the efficiency of laser systems, increase their power, and expand their spectral ranges of generation. The development of new materials for converting laser radiation using methods of nonlinear crystal optics is an urgent problem, as well as the study of their optical properties. Much interest is being directed towards the study of oxide crystals, in particular complex borate crystals. Such crystals, which have been intensively studied in recent years, include huntite-type scandium borate with three cations [1].

This work is dedicated to study the optical properties of scandium borates with the general formula $RE_xPr_ySc_{2+z}(BO_3)_4$ ($x + y + z = 2$, RE = Nd, Sm, Tb, Tm, Yb), grown by the TSSG method. The structure, absorption and luminescence of these crystals have been investigated. The efficiency of second harmonic generation (SHG) of a nanosecond Nd:YAG laser radiation (1064 nm, 6 ns) was studied using the Kurtz-Perry powder technique [2]. The effective nonlinear optical coefficient is estimated at $d_{eff} = 0.34, 0.74, 0.82, 0.85, 0.84$ pm/V for R = Nd, Sm, Tb, Tm and Yb respectively. The influence of the composition and linear optical properties on the efficiency of SHG has been discussed.

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Y-17

INDUCED ABSORPTION SPECTRA OF CRYSTAL VIOLET IN VARIOUS SOLVENTS

N.G. Dmitrieva^{1,2}, O.N. Tchaykovskaya¹, E.N. Bocharnikova¹, and D.M. Ezhov¹

¹Tomsk State University, 36 Lenin Ave., Tomsk 634050, Russia;

²Siberian State Medical University, 2 Moskovsky Trakt St., Tomsk, 634055 Russia, brjantseva@rambler.ru

The study of the triplet triplet absorption capacity of crystal violet (CV) in various solvents was carried out by the pump probe method. Water, dimethyl sulfoxide, isopropyl alcohol and ethyl alcohol were selected as solvents. The formation of triplet states in various CV solvents was revealed upon excitation by nanosecond radiation of the 4th and 3rd harmonics of a Nd:YAG laser