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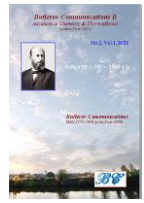

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Quantitative study of the mechanism of interaction of camphor derivatives with cellulose nitrates

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Abstract

This paper presents the results of a study of the features of the physicochemical interaction of cellulose nitrates with camphor derivatives – camphene and carvone. Quantum–chemical calculations of the processes of their interaction were carried out using the HyperChem program. The dipole moments of the starting compounds were calculated, and the individual and mutual solubility was assessed. The nucleophilic and electrophilic properties of cellulose nitrate and modifiers – camphor, camphene and carvone – were determined. The values of the activation energies of the processes of interaction of cellulose nitrates with camphor derivatives were obtained. It was revealed that there is no chemical interaction between them, since the activation energies reach from 1979 kJ/mol to 2882 kJ/mol, and the molecules of the initial substances are not able to overcome such an energy barrier. The fundamental possibility of obtaining heat-resistant composite materials by mixing cellulose nitrate with modifiers (camphor, camphene and carvone) in a common solvent (acetone-diethyl ether) in a ratio of 60%: 40% of the mass is shown. The data of *IR*-spectroscopic studies of modified samples of cellulose nitrates revealed the presence of adsorption on the fibers of cellulose nitrate. X-ray diffraction analysis revealed that modifiers contribute to the amorphization of the structure of cellulose nitrate. The results of thermomechanical analysis show that during plasticization of cellulose nitrate with camphor, camphene and carvone, a decrease in the glass transition temperature is observed by about 110 °C, which is characteristic of molecular plasticization. The data of physical and mechanical analysis confirm this

plasticization mechanism and indicate that the addition of a modifier increases the mobility of cellulose nitrate molecules, which leads to an increase in elasticity and a decrease in the strength of the material and the modulus of elasticity.

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