A STUDY OF THE ELECTRONIC STRUCTURE OF OCTAVINYLSILSESQUIOXANE AND DENDRON WITH CHROMIUM BASED COMPOUNDS BY X-RAY PHOTOELECTRON SPECTROSCOPY AND QUANTUM CHEMICAL MODELING IN THE DFT APPROXIMATION

© **I. S. Osmushko, V. I. Vovna, V. V. Korochentsev, M. V. Tutov, and N. P. Shapkin**

UDC 539.194

The electronic structure and some features of octavinylsilsesquioxane interaction with sulfene chloride chromium acetylacetonate complex were studied by means of XPS and DFT. According to XPS, spectrum lines have close positions for all the studied compounds, half-width for dendrons not exceeding 2 eV. For octavinylsilsesquioxane, the broader lines appear due to the action of substrate atoms. Chemical composition of a dendron was determined by analyzing the concentrations of atoms in different chemical states and a residual content of chlorine atoms. Chemical bonding between the complex and octavinylsilsesquioxane is provided by the covalent interaction of carbon and sulfur atoms.

Keywords: siloxanes, chelate complexes, chromium acetylacetonate, XPS, DFT, electronic structure.