XES AND QUANTUM CHEMICAL INVESTIGATION OF THE ELECTRONIC STRUCTURE OF PHTHALOCYANINE COMPLEXES $MPcH_{16}$ AND $MPcF_{16}$ WITH M = Cu, Co

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The X-ray spectroscopy and X-ray electron study of the electronic structure of unsubstituted phthalocyanines $MPcH_{16}$ and hexadecafluorophthalocyanines $MPcF_{16}$ with M = Cu, Co is reported. Quantum-chemical calculation of the electronic structure of these compounds was performed. The calculation was used to analyze the metal–ligand electronic interaction in the complexes. The theoretically calculated energy position and composition of the highest occupied molecular orbitals were compared with experimental data obtained from X-ray fluorescence spectra.

Keywords: phthalocyanines, X-ray emission spectroscopy, density functional method, photoelectron spectroscopy.