A STUDY OF THE ELECTRONIC STRUCTURE OF POLYVINYLSILOXANE $(CH_2CHSiO_{1.5})_n$ BY X-RAY PHOTOELECTRON SPECTROSCOPY AND QUANTUM CHEMICAL MODELING IN THE DFT APPROXIMATION

V. I. Vovna, I. S. Os'mushko, V. V. Korochentsev, N. P. Shapkin, and M. V. Tutov

UDC 539.194

The electronic structure of polyvinylsiloxane polymeric chains $(Si_2O_3(CHCH_2)_2)_n$ is studied by X-ray photoelectron spectroscopy and quantum chemistry in the DFT approximation. The binding energy of C and O 1*s* electrons occupying inequivalent positions in the polymer coincides within the experimental accuracy. The binding energies for C and O (284.9 eV and 532.4 eV) and for Si2*p*-electrons (102.7 eV) well agree with the values for related compounds. The experimental data for the binding energy are reproduced in HF and DFT calculations only with the extended 6-311**(*d*) basis set. The highest occupied levels of the polymer are π orbitals of vinyl groups.

Keywords: polymers, siloxanes, XPS, DFT, electronic structure.