# A QUANTUM CHEMICAL STUDY OF GERMANIUM–SUBSTITUENT BONDS IN SUBSTITUTED GERMYLENES

© **N. V. Alekseev and E. A. Chernyshev**

UDC 542.128.1

The spatial and electronic structures of a series of substituted germylene molecules are calculated by DFT and HF methods using the PC GAMESS-Firefly program package. Molecular structures are optimized at the DFT (B3LYP/6-31G(2*d*,*p*)) level; wave functions and topological characteristics of the electron density distribution are calculated in the HF/acc-pvtz approximation. By means of NBO and AIM methods, the main characteristics of Ge–X bonds in these molecules are determined. The Ge–X bonds are shown to be the intermediate type bonds. The energies of these bonds are estimated.

**Keywords:** quantum chemistry, germylenes, AIM method, NBO method.