SPECTROSCOPIC CALCULATION OF THE BOND-DISSOCIATION ENERGY OF CH BONDS IN FLUORO DERIVATIVES OF METHANE, ETHANE, ETHENE, PROPENE, AND BENZENE

L. A. Gribov,[1] I. A. Novakov,[2] A. I. Pavlyuchko,[2] and O. Yu. Shumovskii[2]

UDC 539.194.01

The bond-dissociation energy of CH bonds in fluoro derivatives of methane, ethane, ethene, propene, and benzene is determined by spectroscopic and quantum chemical methods. The spectroscopic values of the bond-dissociation energy of CH bonds are calculated in terms of fundamental absorption bands in the anharmonic approximation by the variational method using the Morse anharmonic basis. The quantum chemical calculations are performed using the 6-311G(3*df*, 3*pd*)/B3LYP basis set. The obtained regularities in variations of the CH bond dissociation energy values upon changes in the molecule structure are discussed.

Keywords: anharmonic calculation, bond dissociation energies, fluoro derivatives, methane, ethane, ethene, propene, benzene.