ASSOCIATES OF METHANOL MOLECULES: QUANTUM-CHEMICAL CALCULATIONS OF STRUCTURE AND VIBRATIONAL SPECTRA

I.Yu. Doroshenko, O.I. Lizengevych, V.E. Pogorelov, L.I. Savransky

Taras Shevchenko Kyiv National University,
Faculty of Physics
(*6, Academician Glushkov Prosp., Kyiv 03127, Ukraine*)

S u m m a r y

The character of molecular associations in liquid methanol is studied by quantum chemistry methods. The approximation of density-functional theory with the hybrid exchange-correlation potential B3LYP and atomic basis 6-31G (*d*,*p*) is used. The energy of formation and optimal spatial structure for an isolated molecule and associations of two, three, and four molecules of methanol are calculated. It is found that the sole stable form of a cluster in methanol is the cyclic one. The frequencies and intensities of vibrational Raman spectra are calculated in the harmonic approximation. They are in good agreement with experimental data.