VIBRATIONAL SPECTRUM OF *p*-AMYLOXYBENZYLIDENE-*p*-TOLUIDINE IN THE CRYSTALLINE PHASE

V.Ye. Pogorelov, V.P. Bukalo, I.M. Zhovtobriukh

Taras Shevchenko National University of Kyiv,
Faculty of Physics,
(*2, Prosp. Academician Glushkov, Kyiv 03022, Ukraine; e-mail: pvye@ukr.net*)

S u m m a r y

The Raman spectrum of *p*-amyloxybenzylidene-*p*-toluidine (ABT) liquid crystal in the crystalline phase has been analyzed. The spectrum was recorded in a spectral range of 0–1650 cm^{-1} and at room temperature ($T = 293$ K). The quantum-chemical computer simulation of a molecular geometry has been carried out, and the vibrational frequencies of ABT molecules have been calculated by applying the B3LYP/6-31G(*d,p*) method. The results of quantum-chemical computer simulation were used to interpret the experimental Raman spectrum. The conformational parameters of ABT molecules in the crystalline phase have been determined.