

## Vibrational Spectra of the 2-, 4-Bromo- and 4,4'-Chlorobenzophenones and Their Interpretation Using Structural-dynamical Models

L.M. Babkov<sup>1</sup>, N.A. Davydova<sup>2</sup>, K.E. Uspenskiy<sup>1</sup>

<sup>1</sup>Saratov State University, Moskovskaya st, 155, Saratov, 410012, Russia

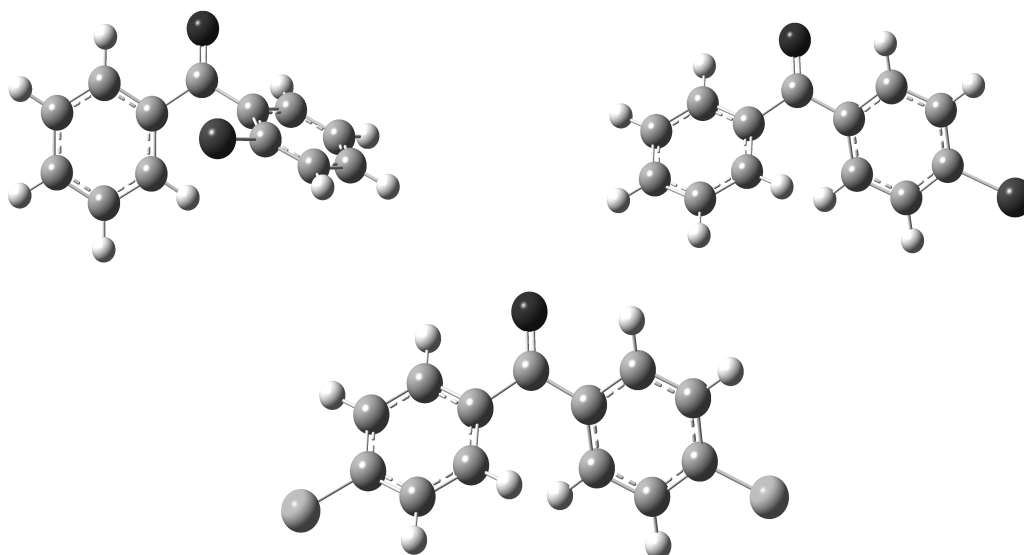
E-mail: babkov@sgu.ru

<sup>2</sup>Institute of Physics of NAS of Ukraine, 46 Nauki prosp., Kyiv, 03022, Ukraine

E-mail: davydova@iop.kiev.ua

In the last time to the investigation of physcal-chemistry properties and the structure of haloido-substituted benzophenones is paid a lot of attention. Between of the investigation methods of these compounds the theoretical and experimental methods of the molecular spectroscopy and quantum chemistry are useful.

Using density functional method (B3LYP/6-31G) [1] the energies, structures, dipole moments and polarizabilities of the 2-, 4-bromo- (2BrBP, 4BrBP) and 4,4'-chlorobenzophenones (4,4'-CIBP) molecules were calculated. In harmonic and anharmonic approximation the force fields of the mentioned above molecules were built and the frequencies of the fundamental normal modes, their forms and intensities in the vibrational spectra together with overtones and combinational frequencies were computed. The comparison of the calculated and measured frequencies pointed to the significant improvement of the modeling results at the transition from harmonic approximation to the anharmonic one. It has been found that it is possible to avoid the scaling procedure for the calculated force fields and vibrational frequencies. On the basis of the modeling results a full interpretation of the measured spectra of the crystalline samples of investigated compounds was given.



[1] J. Frisch, G.W. Trucks, H.B. Schlegel et al., Gaussian03, Revision B.03; Gaussian, Inc., Pittsburgh PA, 2003.