IR SPECTRUM AND STRUCTURAL DYNAMIC ANHARMONIC MODEL OF 2-BENZYLPHENOL

L.M. Babkov1, N.F.Davydova2, M.D. Moskvitin1, J. Baran3
1- Saratov State University, Saratov, Russia
2 – Institute of Physics NAS of Ukraine, Kiyv, Ukraine
3-Institute of Low Temperetures and Structure Research, PAN, Wroclaw, Poland
e-mail: lmbabkov@ gmail.com

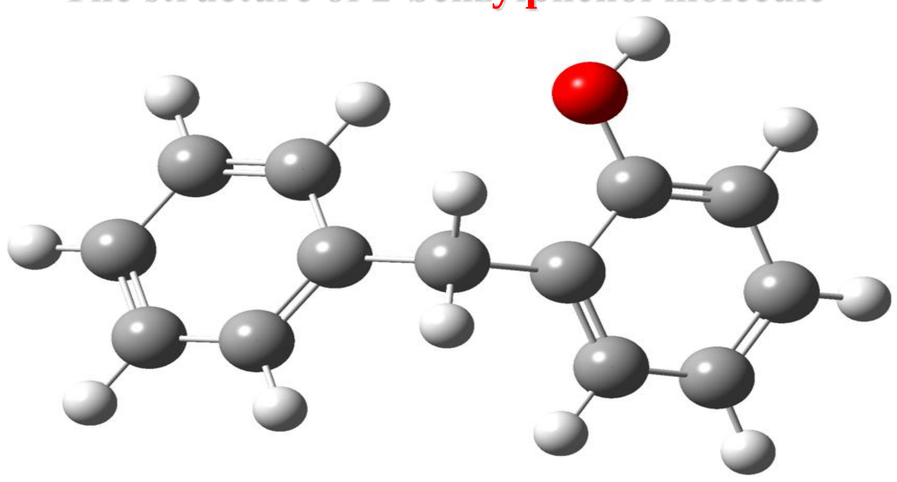
Purpose of the research — **assessment of influence anharmonicity on the calculated IR spectrum of the 2-benzylphenol.**

Tasks – **construction of a structural-dynamic model of a 2-benzylphenol molecule, interpretation of the experimental IR spectrum.**

Research methods – **vibration IR spectroscopy (experiment, theory), density functional theory method (B3LYP/6-31 G(d)).**

RESULTS

The structure of 2-benzylphenol molecule

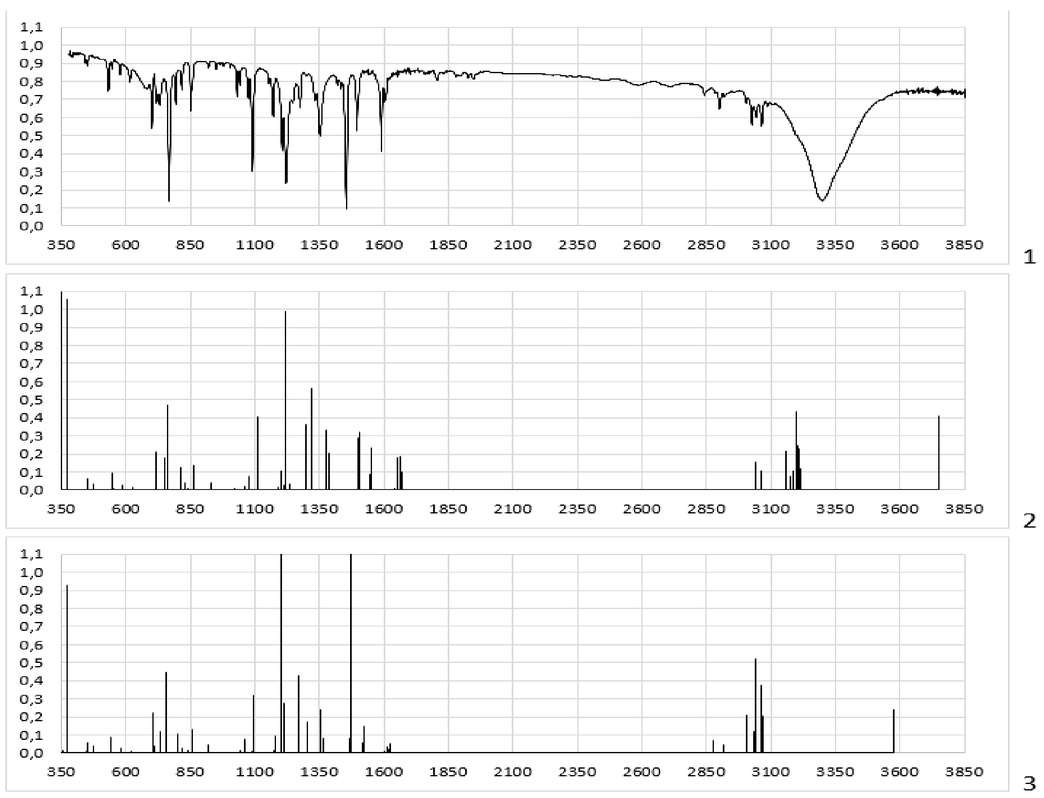


The main parameters of the molecule

Minimum energy: - 577, 8314631,3 Hartree

Bonds length:
O-H – 0,97 Å
C-H ring **- 1,09 Å**
C-H CH2-group **- 1,10 Å**
C-C ring **– 1,39 – 1,41 Å**
C-C single **– 1,52 Å**

Dipole moment – 1, 266 Debye



IR spectra of 2-benzylphenol: experimental (1, stable phase), theoretical (2–harm.), (3- anharm.)

Fragments of the measured and calculated IR spectra od 2-benzylphenol

IR spectra of 2-benzylphenol: experimental (1, stable phase), theoretical (2–harm.), (3- anharm.)

CONCLUSIONS

The construction of a structural-dynamic model of the 2-benzylphenol molecule in the anharmonic approximation made it possible to bring the calculated IR spectrum of the molecule closer to the measured spectrum of the sample and to avoid the procedure of scaling the calculated frequencies, which improves their agreement with the measured frequencies, but has no of physical meaning.