MODELING OF STRUCTURE AND IR SPECTRA OF DIHYDROXYBENZOIC ACID ISOMERS

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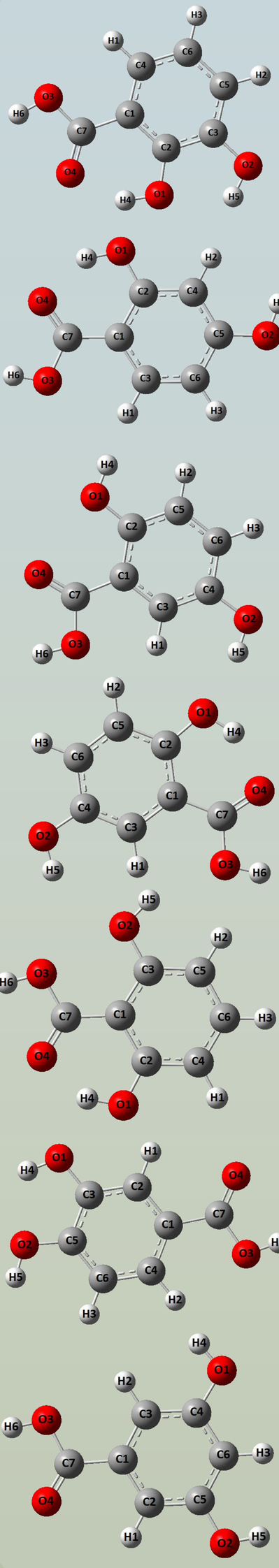
The purpose of work: study the influence of the position of hydroxyl groups relative to the phenyl ring on the IR spectra of dihydroxybenzoic acid (DHBA).

Tasks: construct structural-dynamic models of DHBA isomers and, on the basis of the results obtained, to interpret the measured IR spectra.

Methods: DFT method and functional and basis sets are B3LYP/6-31G(d)

Results of modeling and calculated IR spectra of DHBA



2,3-DHBA
Energy*:
E = -571,2685849
Dipole moment*:
μ_o = 1,886
μ_x = -1,5867
μ_y = 1,0195
μ_z = -0,0012

2,4-DHBA
Energy:
E = -571,2705384
Dipole moment:
μ_o = 1,0297
μ_x = 0,6844
μ_y = -0,7694
μ_z = 0,0005

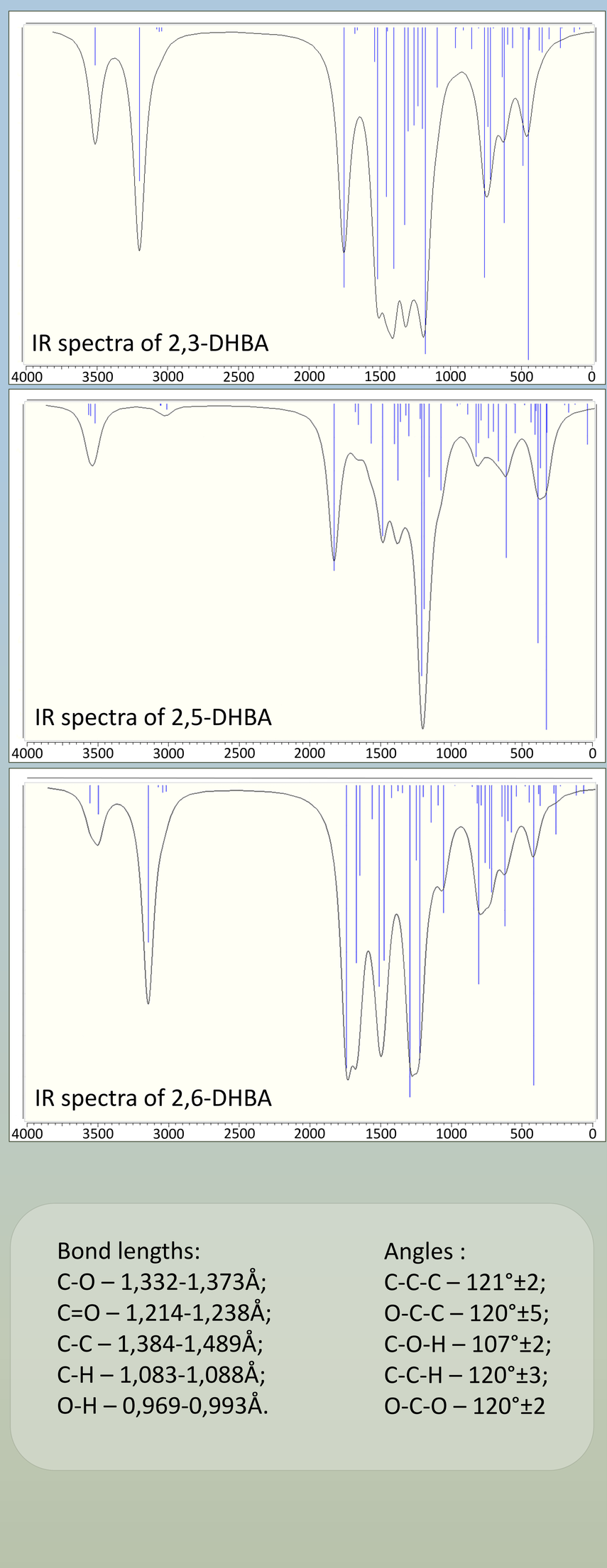
2,5-DHBA
Energy:
E = -571,2448924
Dipole moment:
μ_o = 1,8794
μ_x = 1,8581
μ_y = 0,2821
μ_z = -0,0057

Conformer of 2,5-DHBA
Energy:
E = -571,2637422
Dipole moment:
μ_o = 2,8543
μ_x = -0,2506
μ_y = -2,8433
μ_z = 0,0011

2,6-DHBA
Energy:
E = -571,2615788
Dipole moment:
μ_o = 3,2432
μ_x = 1,2908
μ_y = 2,9752
μ_z = -0,0001

3,4-DHBA
Energy:
E = -571,2560746
Dipole moment:
μ_o = 4,5934
μ_x = -2,4631
μ_y = -3,8772
μ_z = -0,0005

3,5-DHBA
Energy:
E = -571,2540616
Dipole moment:
μ_o = 2,9774
μ_x = 1,3160
μ_y = 2,6708
μ_z = 0,0000



Bond lengths:
C-O – 1,332-1,373Å;
C=O – 1,214-1,238Å;
C-C – 1,384-1,489Å;
C-H – 1,083-1,088Å;
O-H – 0,969-0,993Å.

Angles :
C-C-C – 121°±2;
O-C-C – 120°±5;
C-O-H – 107°±2;
C-C-H – 120°±3;
O-C-O – 120°±2

* energies are in Hartree, dipole moments are in Debye.

Conclusions

1. Based on the results of constructing structural-dynamic models of the isomers of DHBA and the conformer 2,5-DHBA, differences in the vibrational spectra and other parameters of these molecules were revealed, due to the position of hydroxyl groups relative to the phenyl ring.
2. A manifestation of a weak intramolecular hydrogen bond was found in the 2,3-, 2,4- and 2,6-DHBA molecules, as well as in the 2,5-DHBA conformer, which is clearly seen from the intensity peaks in the region above 3000 $см^{-1}$ in the above graphs.