

A Theoretical IR and Raman Spectroscopic Study on 1,2-Bis(o-carboxyphenoxy) ethane molecule

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Salicylic acid is a key molecule in producing of many skin-care products used in the treatment of acne, psoriasis, calluses, corns, keratosis pilaris, and warts. Due to its effect on skin cells, salicylic acid is used in several shampoos used to treat dandruff. Salicylic acid is also used as an active ingredient in gels which remove warts. In our this study subjected to 1,2-Bis(o-carboxyphenoxy) ethane which is a member of the compound group called “Glycol Podands with salicylic acid end”, theoretically possible stable conformers of the molecule in electronic ground state were searched by means of molecular dynamics calculations. The equilibrium geometrical parameters for the determined 19 stable conformers of the free molecule were obtained through geometry optimizations carried out using B3LYP hybrid DFT method with 6-31G(d). The vibrational normal modes and corresponding wavenumbers, IR and Raman intensities for the most stable three conformers of the molecule were obtained by means of frequency calculations performed in “harmonic oscillator” approach at 6-31G(d), 6-31++G(d,p) and aug-cc-pvTZ basis sets.

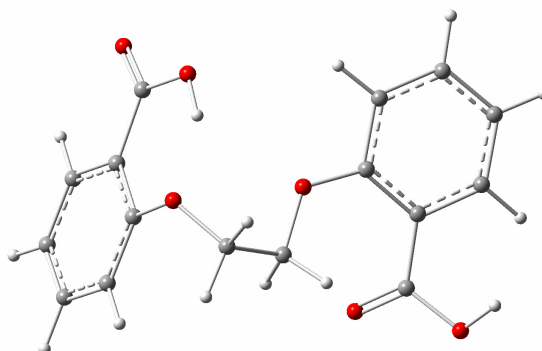


Fig. 1: 1,2-Bis(o-carboxyphenoxy) ethane molecule.

In order to reduce systematical overestimations at the calculated harmonic wavenumbers and thus to fit them to the corresponding experimental wavenumbers, two different scaling procedures referred to as “Scaled Quantum Mechanical Force Field (SQM FF) methodology” [1, 2] and “Scaling wavenumbers with dual scale factors” [3] were proceeded, independently. The obtained scaled wavenumbers have been found to be in good agreement with our assignments proposed for the fundamental bands observed in the recorded experimental IR and Raman spectra of the molecule.

[1] G. Rauhut, P. Pulay, J. Phys. Chem. 99 (1995) 3093.

[2] G. Rauhut, P. Pulay, J. Phys. Chem. 99 (1995) 14572.

[3] M.D. Halls, J. Velkovski, H.B. Schlegel, Theor. Chem. Acc. 105 (2001) 413.