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NUMERICAL SIMULATION OF THE IR SPECTRA OF CARBOXYLIC ACIDS

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ABSTRACT

Our present work reports the IR spectra of carboxylic acids, viz., formic, acetic and benzoic acid monomers recorded by FTIR spectrometer and also simulated theoretically. The simulations were performed at AM1 level using the MOPAC and G F matrix method. In this work following steps were taken: optimizing the geometry, computing the IR spectra and comparing it with experimental spectra. Assuming C_s point symmetry, vibrational assignments for the observed frequencies have been proposed. The spectra exhibit distinct features originating from low frequency vibrational modes caused by intra-molecular motion.

Key words : Benzoic acid, Acetic acid, Formic acid, FTIR spectra, MOPAC, Vibrational spectra.

Carboxylic acids (RCOOH) contain a common and important functional group and provide the point of success to the carboxylic acid derivatives (acetyl chlorides, esters, amides etc.). Carboxylic acids are the most acidic of the common organic functional groups.

Molecular structures and inter/intra molecular interactions have a direct influence on the type of structural framework that biomolecules can adopt. Understanding of fundamental processes, dynamics, molecular-orbital studies and force constants calculations are, thus, main objectives of spectroscopists. Intramolecular force field helps us by identifying fundamental frequencies, assigning fundamental frequencies to correct mode of vibrations, determining reliable force constants and designing the drug as input parameters and to predict vibrational frequencies of related molecules.

Benzoic acid is the simplest aromatic carboxylic acid containing carboxyl group bonded directly to benzene ring[1]. It naturally occurs in many plants and resins. It is also detected in animals.

Carboxylic monomers and dimmers are the simplest models for studying hydrogen bonded systems[2,3,4,5] and they are of utmost importance as doubly bonded hydrogen atoms are abundant in nucleic acid base pairs that hold together the double stranded helices in DNA[6].

In present study, we compared experimental results with calculated frequencies of acids using force matrix method and MOPAC method using AM1 precise. This method was able to account breadth of spectrum as well as description of vibrational modes to encourage the application of a similar procedure to a larger and more complex groups.

Theoretical Calculation :

In noncomplex molecules, the G F Matrix is given by:-

$$G_{tt'} = \Sigma^{3N}_{i=1} (B_{ti} B_{t'i'}) 1/ m_i$$

where t, t' = 1,2,3,……, 3N-6

In which m_i is the mass of the atom to which the subscript I refers and B_{ti}, $B_{t'i'}$ are constants determined by geometry of molecule.

Internal coordinate S_t are related with Cartesian displacement coordinate ξ_i as :

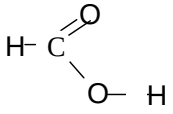
$$S_t = \Sigma^{3N}_{i=1} B_{ti} \xi_i$$

where t = 1,2,3….., 3N-6

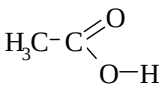
On solving G.F. matrix for any atom α is obtained as:

$$G_{tt'} = \Sigma^{3N}_{\alpha=1} \mu_\alpha S_{t\alpha} . S_{t'\alpha}$$

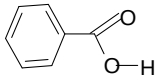
Where dot represents the scalar product of two vectors and $\mu_\alpha = 1/m_\alpha$, the reciprocal of the mass of atom α.



Formic Acid Monomer



Acetic Acid Monomer



Benzoic Acid Monomer