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Research Paper :

Numerical simulation of the internal vibrations of NH_2 in amino-benzoic acids

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ABSTRACT

Our present work reports the IR spectra of amino substituted Benzoic Acids recorded by FTIR spectrometer and also simulated theoretically. The simulation was performed using GF matrix and AM1, PM3, DFT 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 : o-amino benzoic acid, m-amino benzoic acid, p-amino benzoic acid, FTIR spectra, vibrational spectra, AM1, PM3, DFT,G-F Matrix

Carboxylic acids (RCOOH) are a common and important functional group and provide the point of success to the carboxylic acids derivatives (acetyl chlorides, esters, amides etc.). Carboxylic acids are the most acidic of the common organic functional groups. Amino benzoic acid is used by topical application as a sunscreen agent. Amino benzoic acid and its derivatives effectively absorb light throughout the UVB range but absorb little or no UVA light. Amino benzoate sunscreen agents, therefore, may be used to prevent sunburn[7].

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 constant 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. Theoret[8] studied the IR spectra of o-, m- and p-amino benzoic acids in different crystalline forms

With the availability of powerful computers and the advent of efficient density functional theory (DFT) methods implemented in standard codes, structure and dynamics of systems containing a few tens of atoms (or even more) are now within reach. Vibrational spectra of small molecules of biological or pharmaceutical relevance are routinely treated combing DFT electronic structure calculations with a harmonic analysis[9]. Due to deficiencies of the quantum chemical calculations and/or due to the neglect of anharmonic effects, these frequencies are typically a few per cent higher than the observed ones.

We compared experimental results with calculated frequencies of amino benzoic acids using force matrix method and AM1, PM3 and DFT method. These methods were 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 group.

MATERIALS AND METHODS

Amino Benzoic acid were purchased from Sigma Chemical Co (USA). I.R. Spectrum has been recorded in the liquid phase in the range 400-4000cm^{-1} on Perkin-Elmer spectrometer Model 397.

Preparation of KBr Pallets: A small amount of finally grounded solid sample was intimately mixed with about 100 times or more than its weight of Potassium bromide powder. The finally grounded mixture was than pressed under very high pressure in a press (about 10/cm^2) to form a small pallet (about 1-2 mm thick and 1cm in diameter).

The accuracy of the measurements was estimated to be within 3cm^{-1} and the resolution was better then 2 cm^{-1} through the entire range for both the spectra.

Computational and theoretical details :

In noncomplex molecules, the G F Matrix [13] is given by:

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