

Vibrational, NMR and DFT Investigations of Ethylenediaminetetraacetic acid

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Molecular recognition process is the result of several weak noncovalent bonds, due to electrostatic, van der Waals, hydrogen bonding, aromatic π bonds and hydrophobic interactions, having a key role in many important biological reactions. Moreover, the molecular recognition properties exhibited by different molecules can particularly be used for chelation therapy.

Ethylenediaminetetraacetic acid, more commonly known as EDTA, forms complexes with divalent and trivalent metals. The important part of the compound involved in complexing with the metal are the four carboxylic acid groups and the two nitrogens. EDTA is usually administered as a calcium or zinc salt because EDTA has a high affinity for these metals. When EDTA is presented in a Ca or Zn salt form, it not bind these essential metals as highly as when it is administered in the non-salt form. EDTA is also most commonly used for lead poisonings.

The molecular vibrations of EDTA were investigated by ATR FT-IR and FT-Raman spectroscopies. In parallel, quantum chemical calculations based on Density Functional Theory (DFT) are used to determine the geometrical, energetic and vibrational characteristics of the molecule.

The vibrational spectrum of the EDTA has been assigned based on DFT calculations at B3LYP level of theory using the standard 6-31G(d) basis set. The experimental vibrational bands were assigned to the calculated normal modes and a very good correlation was achieved between the experimental and theoretical data. The molecular electrostatic potential of the molecule has been calculated and used for predicting site candidates of electrophilic attack.

The ¹H and ¹³C NMR spectra of EDTA were obtained in DMSO solution and they were also calculated using the GIAO (Gauge-Including Atomic Orbitals) method implemented in the Gaussian package. Again, a very good correlation was found between experimental and theoretical NMR data and this allows us to validate the calculated structure and geometrical parameters of the molecule.

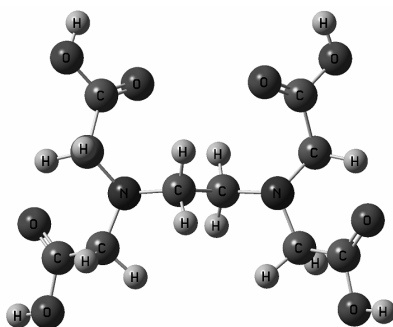


Fig. 1: Optimized molecular structure of EDTA.