FT –IR AND FT RAMAN SPECTROSCOPY STUDY OF VIBRATIONAL ANALYSIS OF DIETHANOLAMINE

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Abstract: The vibrational frequencies and corresponding normal mode assignments of diethanolamine have been calculated using ab initio density functional theory (B3LYP) method with 6-311++G(d,p) basis set level on the ground state. Structural and spectroscopic investigations of diethanolamine were reported. Infrared wavenumbers, infrared intensities were predicted. Calculated infrared wavenumbers and intensities were compared with FT-IR spectra of diethanolamine, supporting for a general assignment of the recorded spectra. The used scale factors which have been obtained the ratio of the frequency values of the strongest peaks in the calculated and experimental spectra seem to cause the gained vibrations well corresponding to the experimental ones. Infrared wavenumbers and their intensities of diethanolamine have been determined. There is an excellent agreement between experimental and theoretical infrared wavenumbers in the region of (4000-400 cm^{-1}). In order to compare of this agreement,. The correlation value of diethanolamine and triethanolamine are found to be 0.9912, 0.9988, respectively for B3LYP method with the 6- 311++G(d,p) basis set.

Keywords: Diethanolamine, DFT, Ft-IR spectrum, Vibrational assignment.

INTRODUCTION

The aromatic amine ligands have been incorporated into various biologically important compounds. A wide variety of aromatic amine derivatives of divergent commercially important compounds have been used as a component in detergent formulations for laundry and dishwashing, degreaser, multiple use detergents and disinfectants (Esker et al., 1999). Ethanolamine derivatives are a class of organic molecules containing amine and alcohol groups. Like other amines, diethanolamine act as a weak base due to the lone pair of electrons on the nitrogen atom (Karadag et al., 2001). Ethanolamine derivatives are also versatile ligands the readily from coordination compounds with almost all metal ions and behave as N and O donor ligand (Bombicz et al., 1997).

Homo and heterobimetallic ethanolamine complexes of a number of metals have been reported recently (Bradley et al., 1978; Kessler et al., 1994; Sen et al., 1970; Brannon, et al., 1971; Mikulski et al., 1987; Umpathy, et al., 1985; Begum, et

., 1994; Yesilel et al., 2007; Yesilel et al., 2004; Uçar et al., 2004 a,b).

This paper is entirely devoted to the vibrational properties of diethanolamine and the ground state. Up to our knowledge no DFT calculations and detailed vibrational analysis have been performed on the studied molecules. A detailed quantum chemical study will aid vibrational modes of the studied molecules and comparison the experimental data for these molecules. Density functional theory calculations are reported to provide excellent vibrational frequencies of organic compound if the calculated frequencies are scaled to compensate for the approximate treatment of electron correlation for basis set deficiencies (Handy et al., 1992; Handy et al., 1994; Stephens et al., 1994; Devlin et al., 1995; Lee et al., 1996a,b). Recently DFT is now accepted as a popular post-HF approach for the computation of molecular structure, vibrational frequencies and energies of molecules by the *ab inito* community (Castella-Ventua et al. 1996).

A quantum chemical investigation using DFT techniques with moderately extensive basis sets have also been performed to help in the assignments of the observed frequencies. However,

Experimental Methods

The Infrared spectra of diethanolamine and t were recorded on Perkin Elmer 100 FT-IR spectrometer in the range of 4000-400 cm^{-1} (2 cm^{-1} resolution) with a DTGS detector.

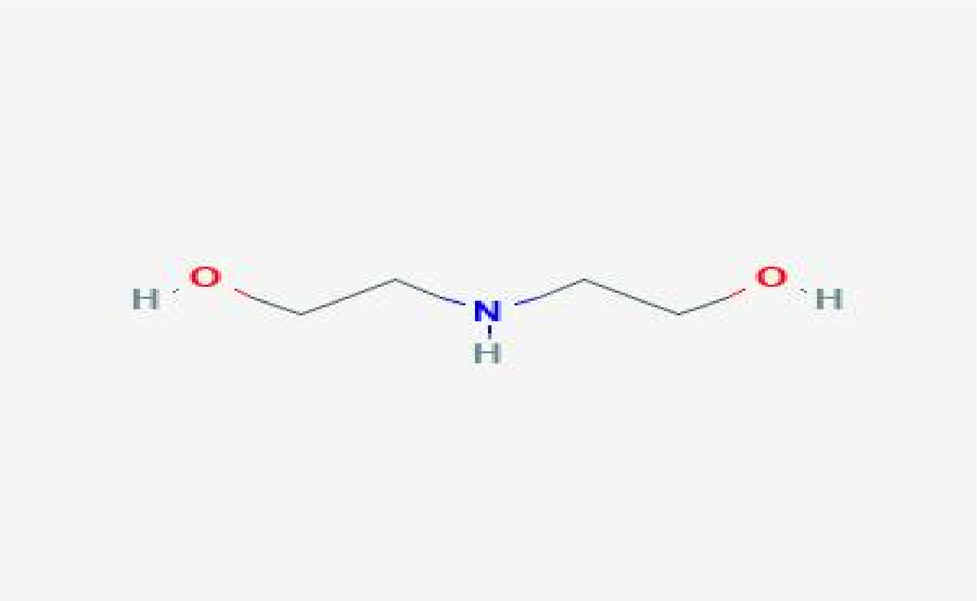
Calculation Methods

Geometry optimizations of the diethanolamine were performed density functional theory (B3LYP). In geometry optimization, the most important parameters that determine the conformation of these molecules are pyramidal of the N atom (measured by the sum of its bond angles and torsional angles of relative to the C-N-C plane). In this study, ab inito calculations were performed utilizing the Gaussian 03 program (Gaussview et al., 2003; Frisch et al., 2004) and carried out at the B3LYP level of theory with 6- 311++G (d,p) basis set. This basis set is a double -type with polarization functions on all atoms to ascertain the importance of diffuse function in the basis on energies and geometries. Electron correlation was treated with density functional theory. The DFT technique employed the Becke3 (B3) (Becke 1992) exchange functional which supplement with Lee, Yang, Parr (LYP) (Lee et al., 1988) correlation functional. The molecular wave function was expanded in a basis of Gaussian functions that represent atomic orbitals. The position of the atomic centre was systematically varied until electronic energy was minimized. In general, electron correlation effects were fairly uniform though a conformational or torsional potential energy surface. Studied calculations on diethanolamine molecules were valuable in order to provide insight into the vibrational spectra and molecular parameters.

RESULT AND DISCUSSION

Geometric Analysis

The molecular structure and atomic numbering for the present study is shown in Fig. 1.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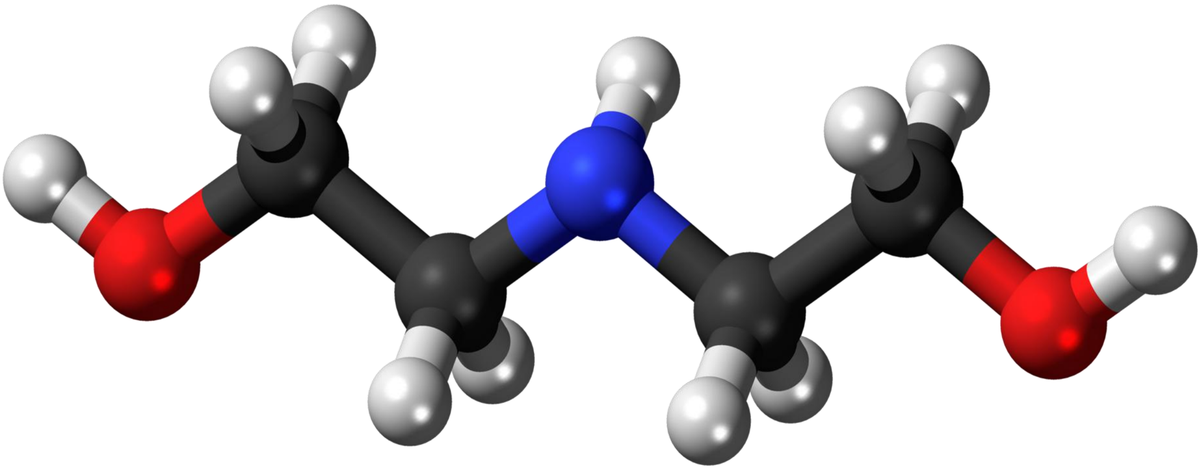
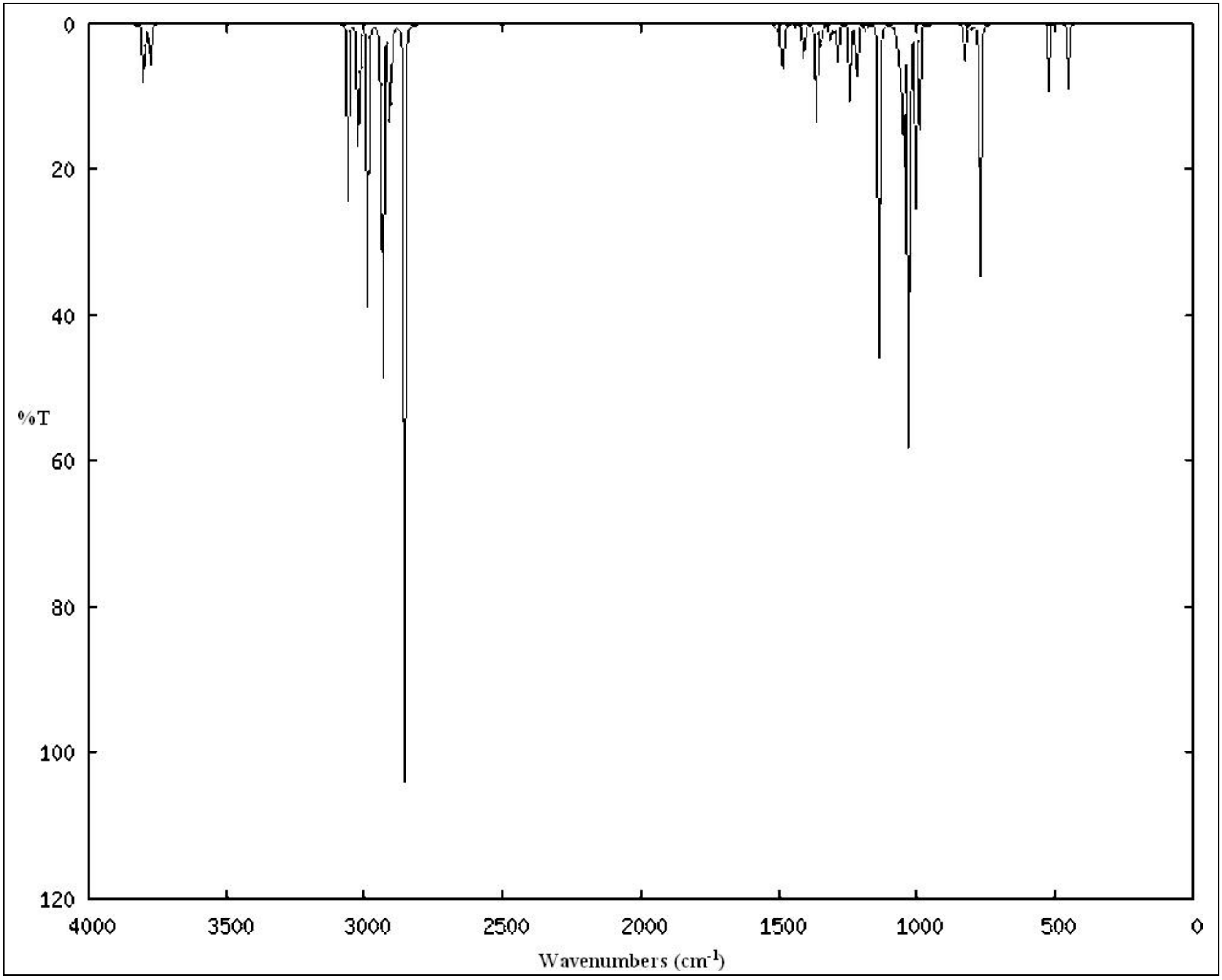


have determined its approximate descriptions with the B3LYP calculation method. The calculated bond lengths for the CN bonds are rather close to the calculated ones for the other, C-NH is included into the influence of electron donating and electron withdrawing in molecular structure of diethanolamine. For comparison, molecular structure of diethanolamine may be compared with molecular structure of triethanolamine. N-C bond lenght is calculated as 1.459Ǻ for diethanolamine . N-C bond lenght is calculated as 1.461Ǻ for diethanolamine . C-O bond angles are calculated as 1.425-
1.427Ǻ for diethanolamine and as 1.426-molecule. C-H bond angles are changed between 1.093 and 1.1 Ǻ for diethanolamine and C-H bond angles are calculated from 1.093 . O-H bond angles are determined as 0.961Ǻ for diethanolamine and changed from 0.961 to 0.968Ǻ molecules.

Vibrational Analysis

Infrared wavenumbers and their intensities were carried out and no negative frequencies are obtained, which indicates that the molecules are in the minimum of the potential energy surface. Both experimental and calculated infrared wavenumbers are tabulated in Table 2 and Table 3

Fig-1 FT-IR SPECTRUM OF DIETHANALOMINE



1.427Ǻ for diethanolamine molecule. C-H bond angles are changed between 1.093 and 1.1 Ǻ for diethanolamine. O-H bond angles are determined as 0.961Ǻ for diethanolamine molecules. A good agreement for bond length on diethanolamine molecules is determined.

Vibrational Analysis

Infrared wavenumbers and their intensities were carried out and no negative frequencies are obtained, which indicates that the molecules are in the minimum of the potential energy surface. Both experimental and calculated infrared wavenumbers are tabulated in Table 2 and Table 3.

Calculated NH bond ise carried out as 3452 cm^{-1} for diethanolamine in this region. Both symmetric and asymmetric fundamental vibrations of CH bonds are calculated as 3062-2853 cm^{-1} and observed as 2930-2847 cm^{-1} for diethanolamine. In plane CH vibration (scissoring, rocking) are calculated as 1507-1480 cm^{-1} and 1299-1286 cm^{-1} for diethanolamine. . Out of plane CH vibration (wagging, twisting) are calculated as 1440-1314 cm^{-1} and observed as 1456-1301 cm^{-1} for diethanolamine. Wagging vibration of CH bond are calculated as 1422-1365 cm^{-1} and observed as 1418-13. In this study we have taken account of symmetric and asymmetric OH stretching of diethanolamine molecules despite of the fact that OH stretching mode could be calculated.

NC stretching are calculated as 1136-1135 cm^{-1} and observed as 1123 cm^{-1} for diethanolamine. The biggest difference between calculated and experimental values of vibrational frequencies of NH bond is reached to be 12 cm^{-1} due to deformation on bond angles of C-N-C because of electronegativity of nitrogen atom. Otherwise, OC stretching is demonstrated well agreement between experimental and theoretical data for diethanolamine molecule.

The overall agreement between theory and experiment is quite reasonable for all methods that we have used. We further found a reliable one-to-one correspon between our fundamentals and any of our calculated frequencies. Lineequations obtained from the graphs in Figure 3, y= 0.9721x+31.279 for diethanolamine . This deviation are shown that experimental fundamentals for B3LYP method.

CONCLUSION

In this study, we've calculated the geetric parameters and vibrational frequencies of the diethanolamine by using B3LYP method with 6-311++ G (d,p) basis set. To fit the theoretical results with experimental ones. There is a superb agreement between experimental and theoretical results. In order to match of this agreement, the correlation graphic supported the theoretical and experimental data has been investigated. The correlation value of diethanolamine is found to be 0.9988. for B3LYP methods with the 6-311+G(d,p) basis sets respectively.

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