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STABILITY ANALYSIS AND STUDY OF ETHYLENE GLYCOL MONOMER AND DIMER COMPLEX

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ABSTRACT: A detailed theoretical study of ethylene glycol molecule have been performed by Hartree Fock (HF) method, second-order Møller-Plesset perturbation theory (MP2), and density functional theory (DFT) using 6-311++G(d,p) basis set. Geometrical parameters, interaction energies, deviation of potential energy curves of hydrogen bonded O–H from that of free O–H, and charge transfer have been studied to analyze stability and nature of hydrogen bond formation molecule of ethylene glycol dimer complex.

KEYWORDS: ethylene glycol, monomer, dimer, interaction energy, frequency, charge transfer, distance of atoms.

INTRODUCTION

Ethylene glycol is applied extensively as drag delivering medium in medical industry and gas hydrate inhibitor in petroleum industry. Experimental study of ethylene glycol molecule and

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ethylene glycol aqueous solution has been performed using nuclear magnetic resonance (NMR) spectroscopy [1], infrared spectroscopy (IR) [2], ultraviolet (UV) spectroscopy [3], Raman Spectroscopy [4], X-ray, and Neutron diffraction techniques [5]. Geometry optimization and interaction energy calculation have been carried out using Hartree Fock (HF) method, second-order Møller-Plesset perturbation theory (MP2), density functional theory (DFT). In the study of molecular complexes in ethylene glycol liquids, the causes of changes in bond lengths, charge transfers, and angles of the monomer and dimer states of the molecule were studied.

Table 1: Ethylene Glycol monomer (Figure-1a) calculated distance of atoms ($d_{X-Y,}$ Å), angle of bonds ($A_{X-Y-Z,}$ degree), atomic charge (q_X, e) using 6-311++G(d,p) basis set.

Parameters	Methods		
	MP2	DFT	HF
$d_{O-H,}$ O_4-H_{10}	0.96	0.96	0.94
A_{H-O-C} H_{10}-O_4-C_2	108.57	108.95	110.32
q_H, H_{10}	0.246	0.267	0.234
q_O, O_4	-0.491	-0.446	-0.511

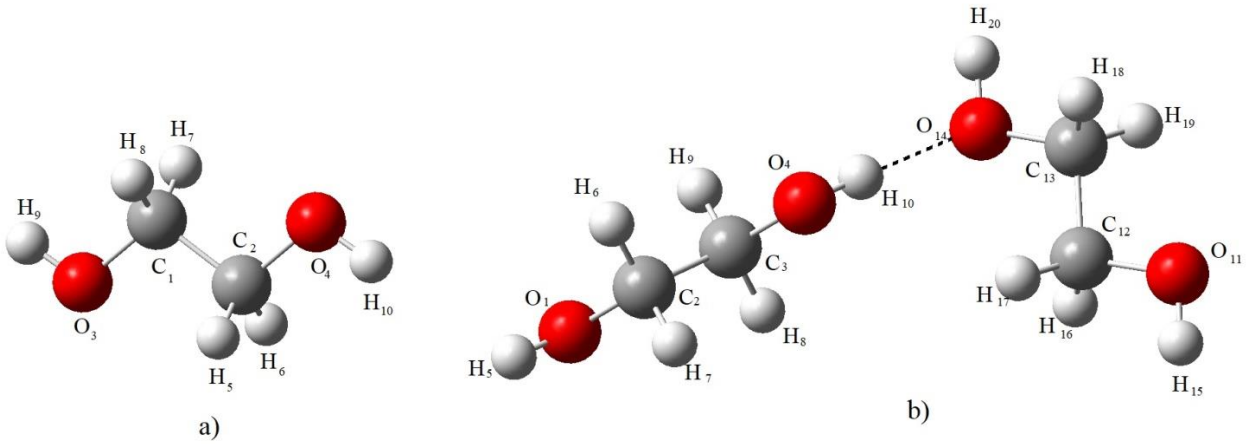

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Figure 1: Optimized structures using B3LYP/6-311++G(d,p) of (a) ethylene glycol monomer, (b) ethlene glycol dimer, (colour legend: red = oxygen, black = carbon, and whitish grey = hydrogen, and black-dotted is hydrogen bond)

Interaction energy (ΔE) for hydrogen-bonded complex is calculated as the difference between the energy of hydrogenbonded complex and the summation of the energies of each component monomer as

$$\Delta E = E_{complex} - \sum E_{components} \quad (1)$$

where $E_{complex}$ and $E_{components}$ optimized energy of hydrogen-bonded complex and each individual component monomer, respectively.

Table 2: Calculated distance of atoms (d_{X-Y}, Å), angle of bonds (A_{X-Y-Z}, degree), atomic charge (q_X, e), hydrogen-bond energy(ΔE, kcal/mole) using 6-311++G(d,p) basis set.

Parameters	MP2	DFT	HF
d_{O-H}, O_4-H_{10}	0.98	0.97	0.97
$d_{O\cdots H}$, $O_{14}\cdots H_{10}$	1.92	1.91	1.91
A_{H-O-C} H_{10}-O_4-C_3	109.06	109.14	110.07
A_{H-O-C} H_5-O_1-C_2	108.76	108.86	109.02
q_H, H_{10}	0.422	0.418	0.409
q_H, H_{20}	0.284	0.289	0.279
q_O, O_4	-0.565	-0.560	-0.558
q_O, O_{14}	-0.522	-0.520	-0.524
ΔE	5.20	5.18	5.17

CONCLUSION

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A thorough analysis of hydrogen-bond formation in ethylene glycol dimer complex has been performed based on interaction energies, potential energy curve for hydrogen-bonded O–H, structural parameters of optimized geometry, and charge transfer.

The bonding energy of the EG molecule in dimer formation is 5.18±0.02 kcal/mole. In the charge distribution, too, the atoms involved in the formation of the hydrogen bond changed significantly more than in the monomer state, depending on the bonding energy in the dimer formation, which can be said to be a medium-hydrogen bond.

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