Global Scientific Review
A Peer Reviewed, Open Access, International Journal
www.scienticreview.com
Volume 22, December 2023 ISSN (E): 2795-4951

The mechanism of formation of molecular conformations in ethylene glycol

Shermatov Abubakir[1], Temurova Elmira[1], Norbutayeva Iqboloy[2], Abduvohidov Sherzod[1] and Elmurzayev Oybek[1]
(Science Supervisor prof.A.Jumabaev)
[1]Samarkand State University of Uzbekistan. [2]Uzbek–Finnish Pedagogical Institute

Annotation

In this work, 4 different tTt, tGg', gTg' and gGg` conformations of the ethylene glycol (EG) molecule were studied using quantum chemical calculations and the method of B3LYP//6-311++G(d, p). Using the calculation, the optical and geometric parameters of the conformations were determined, and at the same time, the change in the shape of the O-H vibration band was analyzed in the conformations.

Keywords: Conformation, interaction energy, charge distribution, hydrogen bonding, Raman spectra

Introduction

Hydrogen bonding is one of the intermolecular and intramolecular interactions that are of great interest to many scientists although its weak interaction. This interaction is present in many compounds in different aggregate states. The study of the nature of hydrogen-bonded compounds using the vibration spectra Raman and IR spectra helps to formulate the theory of hydrogen bonding. No empirical (ab-initio) calculations are currently used to determine the relationship between experiment and theory, as well as to determine the structural properties of the molecule.

The main purpose of this work is to study the mechanism of formation of various conformations in EG molecules and their role in the formation of clusters using quantum chemical calculations. The EG molecule $HOCH_2CH_2OH$ is a biofunctional substance with many applications. EG is widely used in the medical and oil and gas industries, in antifreeze and cooling parts in automobiles, in the melting of ice formed by wind as a result of wind in aircraft, as a moisturizer for fibers and skin. For this reason, this substance is currently being studied in depth using many experimental and theoretical methods [1,2]. Two CH_2OH atomic groups are bonded to their carbon atoms in the EG molecule, and these groups can rotate relative to each other, resulting in definite spatial isomers [3,4]. Since EG has 3 possible rotating dihedral angles, it has 3^3 conformations but 10 of them are the most important. The study of such rotational conformations is important for the study of molecular and intermolecular interactions [5]. Conformations formed in EG molecules have also been studied by many scientists. For example, Yu-Cong Guo [6] et al studied the

monomers of ten conformations of the EG molecule at a temperature of 20 K using FTIR spectrometry and Gaussian–09 program, C. M. Hadad [7] et al studied the EG-water mixture using Raman spectroscopy and DFT theoretical calculation methods. In this study, different conformations of the EG molecule and their different parameters were studied using non-empirical calculations [8]. Imre Bako [9] et al concluded that the formation of dimers of tGg` and gGg` conformations of the EG molecule is stronger than other conformations using non-empirical calculations and the neutron diffraction method. [10] in the study using FTRI and theoretical calculations to study EG in an aqueous medium at a temperature of 198 K revealed that the lines 1033 and 1082 cm^{-1}, corresponding to the C-C stretching vibration mode, belong to the trans- and gauche-conformation. The hydrogen bonds in the EG molecules are broken down in the aqueous medium, and most of the conformations are transformed into transdan- gauche. In this study, 10 different tTt, tTg, gTg, gTg`, tGt, tGg, tGg`, gGg, gGg`, g`Gg` in the dihedral angles H–O–C–C, O–C–C–O and C–C–O–H coformational rotamers have been identified. H. Takeuchi et al studied 3 different deformations of EG in the IR spectra and theoretical calculations using the low temperature argon matrix method. Spectral changes showed the presence of tGg' and gGg' conformations connected by two hydrogen bonds in the O-H vibration field. The role of tTt conformation is also seen in the field of C-O and O-H oscillations [11].

2. Result and discussion

The role of conformations in the study of the mechanisms of clusters within matter is great. We performed calculations to determine the electro-optical parameters of the EG conformations. In Figure 1, 4 types of EG tTt, tGg`, gTg`and gGg` conformations are given. As can be seen from Table 1, the O-H symmetric and asymmetric vibrations of different frequencies correspond to different conformations of the EG molecule.

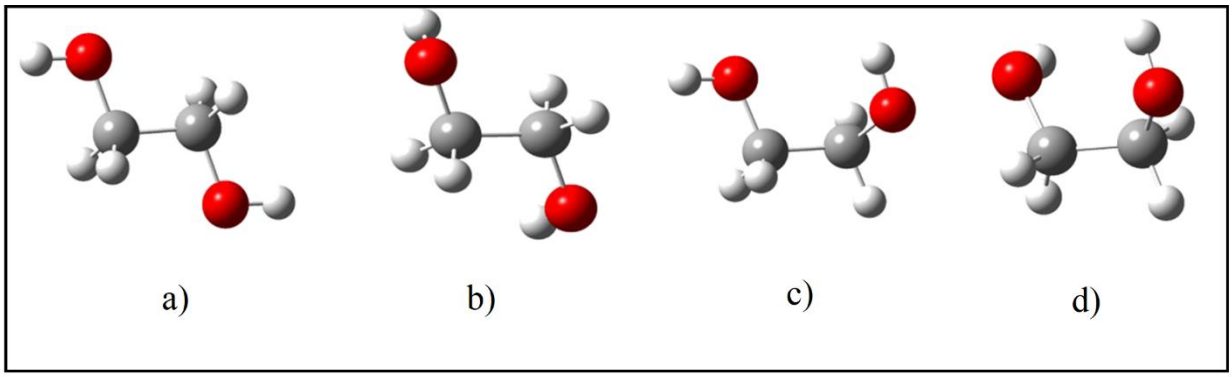

Figure 1. 4 different conformations of EG a) – tTt, b) – gTg`, c – tGg', d) – gGg`

Table 1. O-H symmetric and asymmetric vibration frequencies (cm^{-1}), dipole moment (D), energy of molecule formation (Hartree) and the difference in these energies (kkal/mol) obtained in theoretical calculations of the EG molecule

Conformation	υ_{sim}(O-H)	υ_{ass}(O-H)	Dipole moment	E_o(Hartree)	ΔE(Hartree)	ΔE(kkal/mol)
gTg’	3824	3823	2.5199	-230.3357	0	0
tGg’	3840	3633	2.2741	-230.3393	0.00356	2.3345
tTt	3849	3849	0	-230.3361	0.000366	1.4849
gGg’	3851	3801	2.5095	-230.3403	0.004539	2.8479

As can be seen from the table, the dipole moments also differ from each other. The reason for this difference is that in the tTt conformation, which maintains the symmetry of the molecule, the dipole moment is 0, and in other conformations, it has a dipole moment because the symmetry of the molecule is broken. The energy of formation of the molecule E is obtained with respect to the smallest gTg` conformation E, and the largest energy belongs to the molecule of gGg` conformation.

The Raman spectrum is calculated using theoretical calculations of the O-H vibration frequencies of the monomer of the EG molecule (Figure 2).

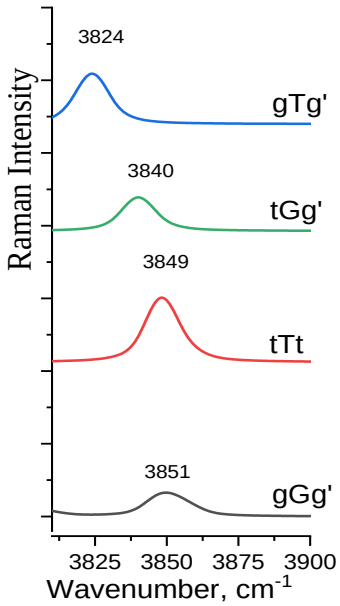

Figure 2. Raman spectra of O-H vibration lines of tTt, tGg`, gTg` and gGg` conformations of EG molecule.

As can be seen from the figure, the frequencies corresponding to the O-H vibration of the EG with respect to the gTg`-conformation, it was observed that the maximum frequencies shifted towards the lower frequency. The largest shift is gTg` -

conformation. Based on theoretical calculations, it can be shown that the O–H vibration line of the conformations tTt, tGg', gTg' and gGg' shifts towards a lower frequency, and the main reason for such a shift is that the molecule has different conformations and different dipole moments in these conformations.

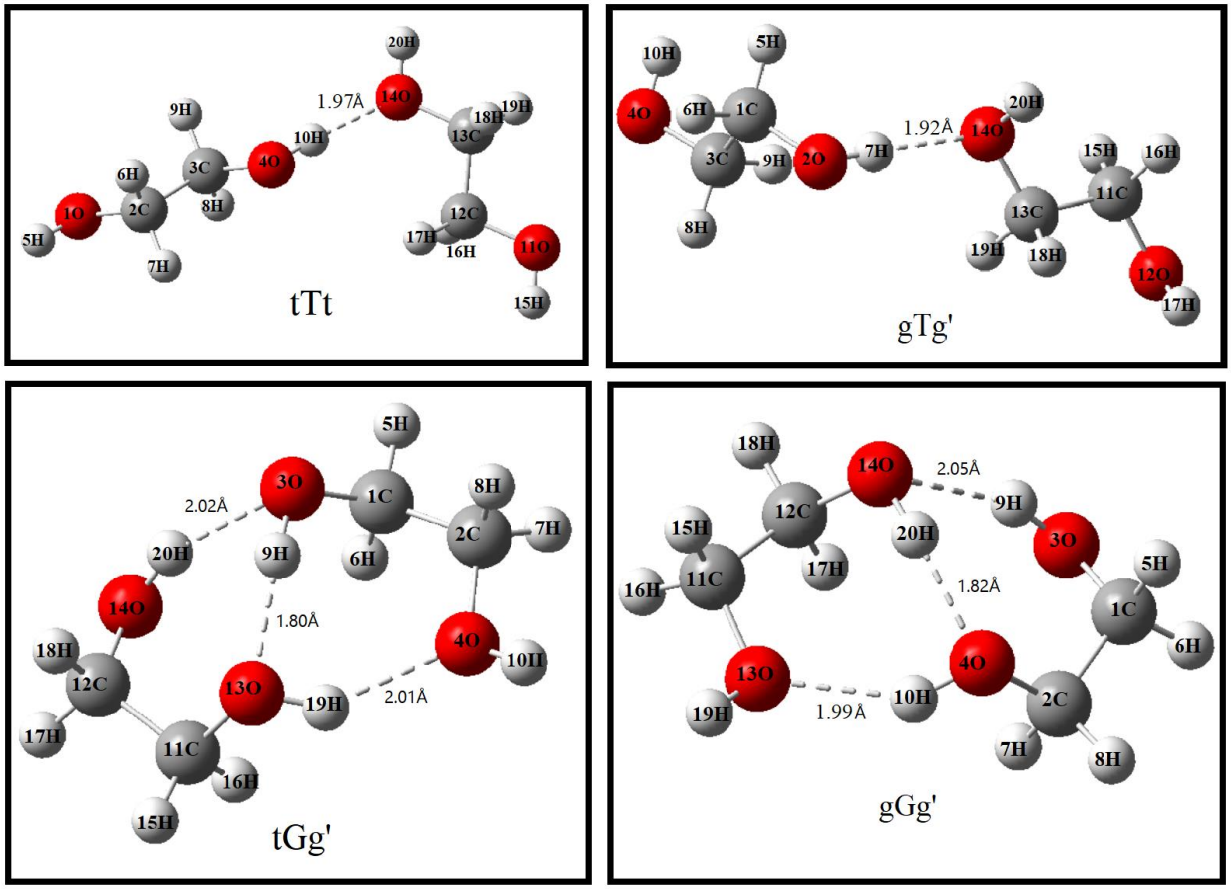

Figure 3. Optimal geometric structure of dimers of tTt, tGg`, gTg` and gGg` conformations of EG molecule.

Figure 3 shows the dimers corresponding to the tTt, tGg', gTg' and gGg' conformations of the EG molecule. The potential of tTt and gTg' conformations in the formation of an open structural dimer of the EG molecule is high, and in the formation of a closed structural dimer is clearly manifested in the conformations tGg' and gGg'. As shown in Figure 3, EG molecules form dimers of different appearances. In the formation of a dimer in the tTt conformation, the H-atom of the O-H group of the first molecule forms a hydrogen bond with the neighboring molecule of the O atom of the O-H group, and these open-type aggregations are observed. The energy of formation of such aggregates is 5.18 kkal/mol.

In the same gTg` conformation, in the formation of the dimer, the first molecule, the H-atom of the O-H group, forms a hydrogen bond with the neighboring molecule, the O atom of the O-H group, and open-type aggregations are formed The energy of formation of such aggregates is 5.33 kkal/mol.

A different picture is observed in the formation of dimers in the gGg`. In this case, the molecules have simultaneously protondonor and protonacceptor properties, forming closed structural aggregates as a result of the formation of 3 different types of H-bonds. The energy of formation of such aggregates is 8.17 kkal/mol.

Table 2. The O-H vibration frequency involved in H-bonding in the formation of dimers ν*, ν O-H vibration frequency not involved in H-bonding, energy of complex formation ΔE(ккал/мол) of the EG molecule

Conformation	$\upsilon^*(sm^{-1})$	υ (sm^{-1})	ΔE(kkal/mol)
tTt	3676	3847	5.18
gTg’	3674	3820	5.33
gGg’	3528 3696 3728	3840	8.17
tGg'	3536 3688 3728	3840	9.39

The formation of dimers in the gGg`conformation is also described above. The energy of formation of such aggregates is 9.39 kkal/mol.

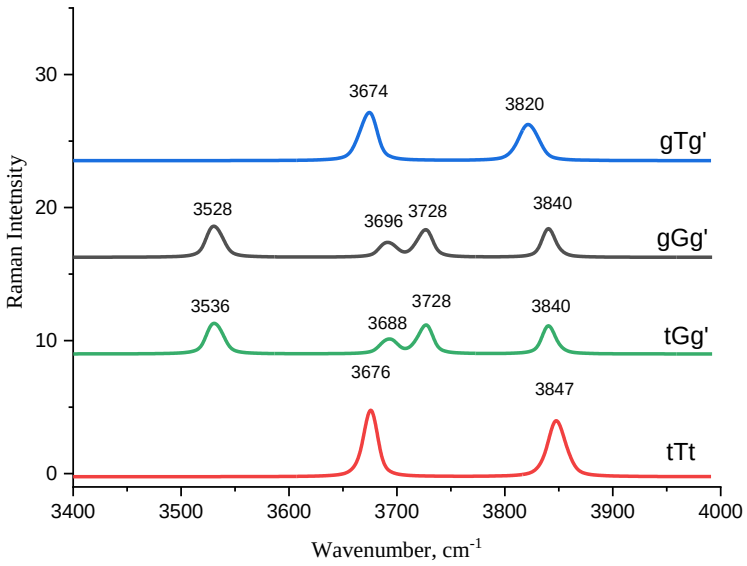

Figure 4. Raman spectrum obtained by theoretical calculations of dimers of conformations tTt, gTg`, tGg` and gGg` of the EG molecule.

Figure 4 shows the vibration line determined using theoretical calculations. It can be observed that in the gTg` conformation there are lines 3820 $cm^{-1}$ and 3674 $cm^{-1}$, the line 3820 $cm^{-1}$ belongs to the O-H vibration, which is not involved in the H-bond, and the line corresponding to O-H vibration 3674 $cm^{-1}$ is involved in the H-bond. In the gGg` conformation, the line 3840 cm^{-1} is the O-H vibration line, which is not

involved in the H-bond, while the line 3728 cm^{-1}, 3696 cm^{-1}, 3528 cm^{-1} is the O- H as long as H belongs to the vibration lines. In the tGg` conformation, the line 3840 cm^{-1} is the O-H vibration line, which is not involved in the H-bond, while the line 3728 cm^{-1}, 3688 cm^{-1}, 3536 cm^{-1} is the O-H it can be seen that H belongs to the vibration lines.

In the tTt conformation, a line equal to 3847 cm^{-1} is an O-H vibration line not involved in the H-bond, while a line equal to 3676 cm^{-1} belongs to the O-H vibration line involved in the H-bond.

Conclusion

- It was found that the spectrum of the EG molecule has different conformations of the molecule to the width of the O-H vibration line and that their O-H vibration lines are different;
- The EG molecule is more active in the formation of closed structural dimers in tGg` and gGg` conformations, and more active in the formation of open structural dimers in gTg`and tTt conformations;
- In the EG molecule is more stable than the gTg' and tTt conformations due to the relatively large binding energy in dimers of tGg and gGg conformations in dimer formation.

References

1. H. Hushvaktov, A. Jumabaev, G. Murodov, A. Absanov, G. Sharifov. Ukr. J. Phys. 2020. Vol. 65, No. 4.
2. M.A. Krestyaninov, A.G. Titova, A.M. Zaichikov. Fiz. Khim. 88,1939 (2014) (in Russian).
3. V.M. Bilobrov. Hydrogen Bond: (Naukova Dumka, 1991) (in Russian).
4. Ye.Vaskivskyi, Ye.Chernolevska, A.Vasylieva, V. Pogorelov, R. Platakyte, J. Stocka, I. Doroshenko. J. Mol. Liq. 278, 356(2019).
5. Jindal, S.Vasudevan, J. Phys. Chem. *B*, Just Accepted Manuscript, Publication Date (Web): 11 May 2017.
6. Y.C. Guo, Ch. Cai, Y.H. Zhang, AIP Conference Proceedings **1725**, 020101 (2016); https://doi.org/10.1063/1.4945555
7. C. M. Hadad, H. C. Allen, E. L. Hommel, J. K. Merle, G. Ma, J. Phys. Chem. B 109, 811–818 (2005).
8. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, at all. *Gaussian 09* (Gaussian, 2009), Re-vision A.02.
9. I.Bako, T.Grosz, G. Palinkasa. J. Phys. Chem. 3215-3221 (2003);
10. Y.C. Guo, C. Cai, Y.H. Zhang, AIP Advances **8**, 055308 (2018), https://doi.org/10.1063/1.4995975
11. H.Takeuchi, M.Tasumi, Chemical Physics 77(1983) 21-34