

Accurate Spectroscopic Characterization, and Formation Pathways of Ethane 1, 1 diol: A Potential Interstellar Molecule

Emmanuel E. Etim^{1*}, Oko Emmanuel Godwin² & Humphrey Sam Samuel¹

¹Department of Chemical Sciences, Federal University Wukari, PMB 1020, Nigeria

²Astrochemistry & Astrophysics Center, Institute of Applied Chemical Sciences, Universidad Autonoma de Chile, Av. Pedro de Valdivia 425, Providencia, Santiago, Chile

Abstract

With exceptions, the correlation between relative energies of isomers and their relative abundances in the interstellar medium (ISM) holds to an extent. Among the C₂H₆O₂ isomers, ethylene glycol is the only known interstellar isomer but there is no report regarding the astronomical searches for ethane 1,1-ethanediol (the most stable isomer of the group) due to lack of spectroscopic and other parameters that would have warranted the search. In this article, the most energetically stable conformer of 1,1-ethanediol was investigated, its spectroscopic, and other parameters are obtained from high level ab initio quantum chemical methods. Accurate spectroscopic parameters are obtained at the CCSD(T) level. The proposed formation route of ethane 1,1-diol has a surmountable barrier considering the nature/abundance of the participating species and the energy sources in ISM. The astrophysical implications of these results are discussed and the astronomical searches of ethane 1, 1 diol are proposed.

Keywords: 1,1-ethanediol, spectroscopic constants, formation pathways, astrochemistry

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***Corresponding author**

E. E. Etim ✉

emmaetim@gmail.com

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Introduction

The interstellar medium (ISM) that was once considered as being chemically barren has now emerged as one of the richest reservoirs of chemically bonded matter in nature with the discoveries of hundreds of different molecular species ranging from the simple diatomic species to the complex molecular species from different regions of the ISM with each discovery telling the story of the physics and chemistry of the environment/region from where the molecular species was discovered. Prominent among these interstellar molecular species are isomers as a good percentage of these molecular species have been detected in more than one isomeric form in the ISM. Thus, the detection of an isomer in the ISM serves as a pointer to the presence and detectability of other isomers in ISM [1, 2, 3, 4].

Though several molecular species belong to the C₂H₆O₂ isomeric groups, ethanediol comes in two isomeric forms which differ only in the placement of the hydroxyl groups. In 1,1-ethanediol, both hydroxyl groups are attached to the same carbon while in 1,2-ethanediol (also known as ethylene glycol) each carbon atom has one hydroxyl group attached to it. The correlation between the relative energies of isomers and their relative abundances in the interstellar medium (ISM) has been well demonstrated. According to the Energy, Stability and Abundance (ESA) relationship “Interstellar abundances of related species are directly

proportional to their stabilities in the absence of the effect of interstellar hydrogen bonding” [3, 4, 5, 6].

Among the isomers of the C₂H₆O group, ethylene glycol is the only known interstellar molecule [7, 8, 9]. However, ethane 1,1 diol is the most stable isomer of the group (please see the figure below) yet it has not been detected. This could be partly due to lack of data as there exists a dearth of information in literature regarding the spectroscopic parameters of ethane 1,1 diol that could warrant its astronomical searches.

Two isomeric forms of ethanediol exist, they differ only in the placement of their hydroxyl group: 1,1-ethanediol and 1,2-ethanediol (ethylene glycol). A structural depiction of the two isomers is shown in Fig. 1 below:

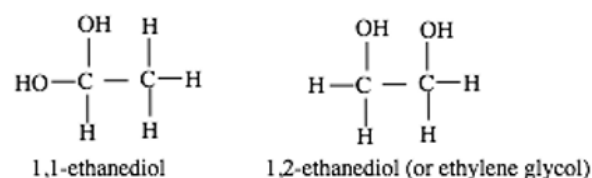


Figure 1: Isomeric forms of 1,1-ethanediol

While both species have the same molecular formula and some physical properties due to the presence of diols, they are all unique in their own way. 1,1-ethanediol, also known as acetaldehyde hydrate is



formed when water is added to ethanal and also has few medical uses (National Center for Biotechnology Information (NCBI)) [10]; whereas 1,2-ethanols is known to have diverse applications such as raw material for polyester fibre manufacturing and as antifreeze [8], its use as a heat transfer fluid has also been reported [11] among other studies on this species such as theoretical studies and fermentation studies [12, 13], respectively.

In addition, findings from recent investigations show that chemical models used for the simulation of molecular abundances fail to accurately reproduce molecular abundances, this findings stem from different comparative studies of the impacts of different reaction pathways on the abundance of some species such as organic acids (formic acids) using observational instruments and models [14, 15, 16]. Consequently, the importance of pathways of formation and destruction has been stressed. Research on chemical evolution of species over time has also been shown tied to knowledge of reaction pathways of the species [17]. By and large, research is necessary to understand the pathways of 1,1-ethandiol which will go a long way in helping model chemists to reproduce its abundance and study its evolution over time.

Among all the possible isomers of this group (C_2H_6O), only 1,2-ethanediol has received wide range of studies and has been detected. However, 1,1-ethanediol, which is more stable suffers obscurity, meanwhile its stability should be a direct pointer to its abundance in the interstellar medium (ISM) and calls for attention. It is pertinent to search for this specie in different environment in the astrophysical environments; however this is difficult without relevant parameters such as the spectroscopic parameters necessary for its exploration. As a result, the current investigation is aimed at providing high level spectroscopic data relevant for this exploration, we also postulate relevant reaction pathways of its formation and destruction, these parameters are vital in understanding the place of 1-1-ethanediol in the ISM and beyond.

Computational Methods

To solve the wavefunction to obtain the needed spectroscopic parameters, we started by defining the molecular geometry, this geometry was optimised at a high level formalism and complete basis set limit; Coupled-cluster single, double and perturbative triples CCSD(T)/CBS(T,Q)+CV(CT), the rotational constants for this structure were also obtained at this level of theory. To ensure that the optimised structure is a true minima, we carried out vibrational analysis of the frequency, the vibrational frequencies were computed at the CCSD(T)/cc-pVTZ level of theory. vibrational corrections at the frozen-core Møller-Plesset perturbation theory at second order (MP2) alongside correlation-consistent polarized valence triple-zeta basis set. fc-MP2/cc-pVTZ level and all these parameters (Spectroscopic parameters) were obtained using the CFOUR program [18, 19, 20]. Conformational analysis

were executed at the DFT level using the B3LYP/6-31g(d,p) level of theory.

Results and Discussion

The optimised geometry, and all relevant spectroscopic parameters and reaction pathways and their implications are presented and discussed. In Fig. 1, we present the isomeric forms of **1,1-ethanediol** and Fig. 2 depicts the five possible isomeric chemical species of the family C_2H_6O , the optimised structure of 1,1-ethanediol is shown in Fig. 3. Accounting for the extent of variation in their energies, the energies illustrated in the Figure are relative to the lowest energy isomer (1,1-ethanediol) for clarity and this range from 11.3 kcal/mol for the already detected specie 1,2-ethanediol (high relative energy) to 17.7 kcal/mol for methoxymethanol, 68.1 kcal/mol for ethylhydroperoxide, and 79.0 kcal/mol for methyl peroxide. We also included their astronomical status in the Figure, respectively.

Accurate spectroscopic characterization, and formation pathways of ethane 1, 1 diol

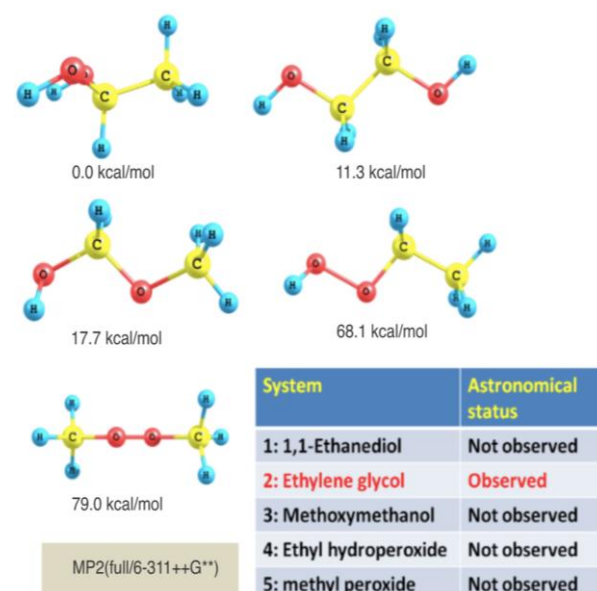


Figure 2: Possible isomers of the general formula C_2H_6O

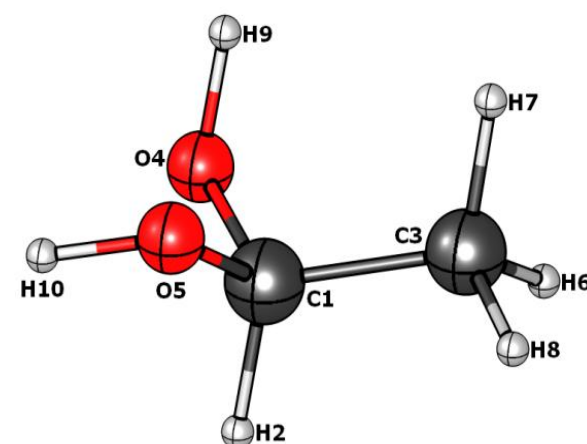


Figure 3: Optimised geometry of 1,1-ethanediol

For ground state 1,1-ethanediol, with 24 degrees of freedom, two of these vibrations correspond to methyl rotation (CH_3 -group of the molecule); (mode 124.3748 and 230.1697) signifying some level of internal rotation in the molecule. The methyl rotation impacts the diols in an inverse method such that when the methyl rotation is higher (mode: 230.1697), the diols have lower twist vibrations and for a lower methyl rotation (mode: 124.3748), the diols have higher twist vibrations. The effect of these can give rise to many observations like diverse conformations which can then influence its chemical reactivity, it can as well impact its rotational and infrared spectra leading to splitting of the spectral lines) [21, 22].

To ascertain this, it is imperative to carry out a conformational analysis of this species. This analysis as presented in Fig. 4 revealed that a more stable conformer (rotamer) of this species exhibits the diols arranged in an adjacent position to each other. Generally, the more stable conformer exhibits staggered

conformation and the OH-groups do not face the same direction and not opposite direction roughly around 90 degrees to each other as shown in the optimized geometry. The analyses illustrate the large difference in energy levels between the most stable conformer and other conformers, this is crucial in spectroscopic characterisation because an attempt at using the unstable isomers for spectroscopic characterisation will lead to the use of unstable structures, the energy level differences is much about 3.62 - 4.01 kcal/mol. Recall that potential energy and stability have an inverse relationship, therefore a conformer with high potential energy is unstable compared to one with low potential energy, more stable. Particularly, these conformers potential energy is accrued from torsional strain (dihedral angles) due to free rotation around the s-bond. It should be noted that both the CH_3 part and diols (two OH groups) all exhibit some form of rotation.

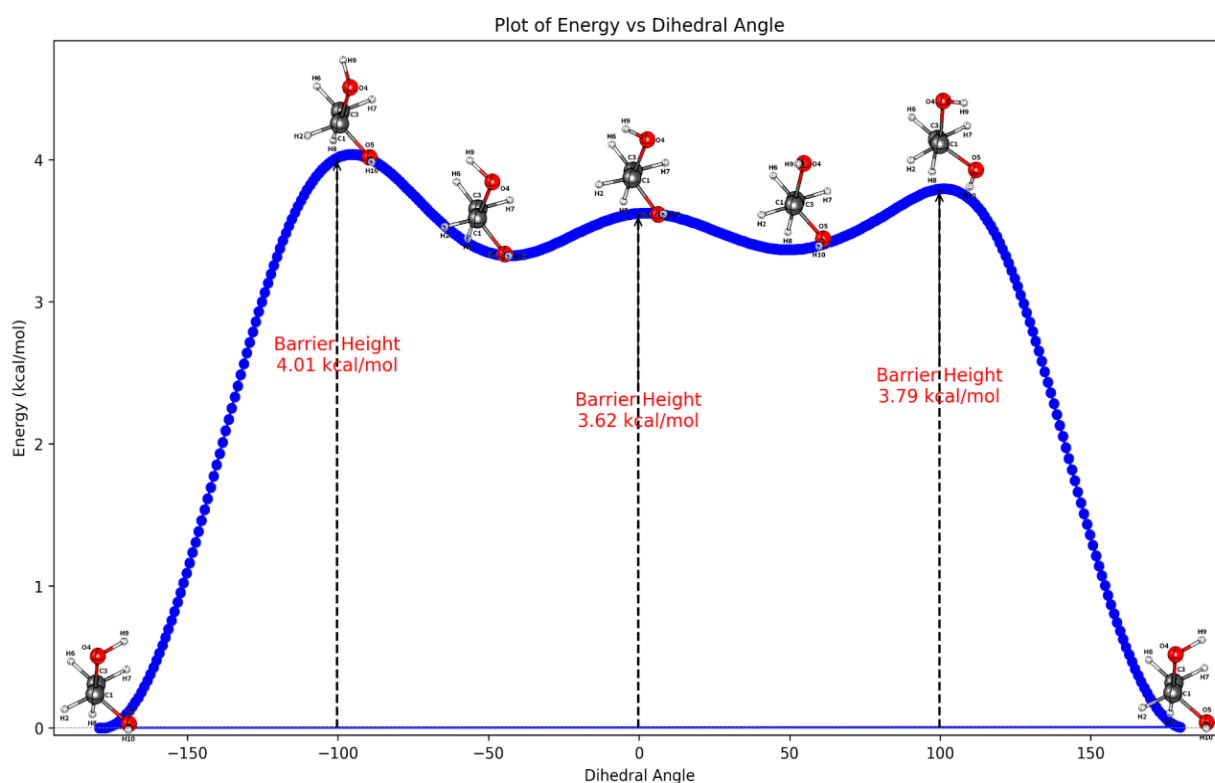


Figure 4: Conformational analysis of 1,1-ethane diol corresponding to the HCOH dihedral

Spectroscopic parameters

Firstly, analysis of the vibrational frequencies enabled the characterisation of the optimised structure as true minima (no imaginary frequency observed). The harmonic and anharmonic vibrational frequencies are given in Table 1 alongside the corresponding infrared (IR) intensity. As a real molecule which deviates from harmonic oscillator approximation, we included the anharmonic vibrational frequencies which takes care of the corrections.

1,1-thandiol shows exhibits vibrational modes characterised as low frequency modes (far IR region), mid-frequency modes (mid-IR regions which spectroscopic explorations of most chemical composition occurs) and high frequency modes (near IR-regions where cool astronomical observations occur), the highest frequency vibrational modes occurs around 1512.5425 to 3669.3244 cm^{-1} indicating the molecule can absorb electromagnetic radiations within the IR windows [23, 24].



Table 1: The vibrational (fundamental) frequencies of 1,1-ethandiol

Irrep	Harm. Frequency	Anharm. Frequency	Harm IR intensity
A	124.3748	87.9982	60.0939
A	230.1697	220.0602	3.7570
A	357.6630	285.1495	134.2250
A	400.2878	395.7318	10.3224
A	458.5896	456.8708	21.4221
A	584.1205	570.6437	9.8586
A	880.5840	864.3075	5.5391
A	962.0955	940.1845	92.1653
A	1056.1378	1035.5719	38.4486
A	1125.5855	1098.6859	50.6241
A	1149.5960	1120.6829	32.5409
A	1242.8308	1195.952	204.9475
A	1303.9783	1287.5547	33.0116
A	1399.0250	1367.578	5.1152
A	1405.5833	1369.1903	6.2224
A	1490.9979	1450.3463	3.3082
A	1497.1352	1452.8879	0.2484
A	1512.5425	1467.8445	25.5091
A	2998.6624	2944.2749	67.9176
A	3059.2755	2955.4673	8.1663
A	3144.1371	3005.6687	16.5893
A	3150.1687	3010.3467	15.3170
A	3844.7460	3668.0357	32.3448
A	3845.4293	3669.3244	11.4400

Harmonic frequencies & intensities at the CCSD(T)/cc-pVTZ level
 Anharmonic frequencies = Harmonic freq (CCSD(T)/VTZ) +
 Anharmonic corr. (MP2/VTZ)

The rotational constants of 1,1-ethandiol are presented in Table 2, It's clear that the rotational constant B is dependent on the molecule's bond length and moment of inertia. As such, rotational constants are relevant to describe the molecular structure vividly. In addition, it can be used to simulate the molecule's rotational spectra, this is relevant for identifying the molecule across diverse environments, this is done by comparing the observed spectra with the simulated or calculated spectra.

The rotational constant when the molecule is in its rest position and considering only rotational motion is represented by the equilibrium rotational constant (e) and when considering the lowest vibrational state, the molecule's structure slightly changes and so we also accounted for that via the inclusion of the ground vibrational state.

Table 2: Rotational constants and centrifugal distortion constants

Rotational constants (MHz)		Quartic Centrifugal dist. constants (KHz)		Sextic Centrifugal dist. constants (Hz)	
Equilibrium rot constant (e)	Ground vibr. state (00)	A-reduced	S-reduced	A-reduced	S-reduced
9225.28	9187.4	DELJ=4.4800	DJ=1.8619	HJ=0.0064994	HJ=0.0269236
8974.85	8848.4	DELK=-1.1311	DK=-14.2214	HJK=-0.2384624	HJK=-0.4744314
5117.55	5069.3	DELJK=5.0574	DK=20.7658	HKJ=0.4755561	HKJ=0.9557565
		delJ=1.6682	dJ=-1.6682	HK=-0.2376554	HK=-0.5023110
		delK=5.8579	dK=-1.3090	hJ=0.0031283	h1=-0.0033960
				hJK=-0.1128581	h2K=-0.0102121
				hK=0.1067195	h3=0.0065243

An obvious analysis shows the ground rotational constant is slightly lower than the equilibrium rotational constants, this is obvious in the sense that, during vibrational motion, the molecule's bond length increases, this leads to an a change in the molecule's moment of inertia thus reducing the rotational constants.

We also included centrifugal distortion corrections at the quartic and sextic levels owing to the fact that a real rotating molecular system experience distortions, thus the asymmetric and symmetrical reduced quartic and sextic corrections are included in the Table.

Possible formation pathways

The following five reaction pathways were proposed and tested;

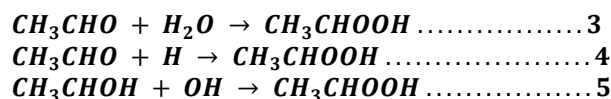
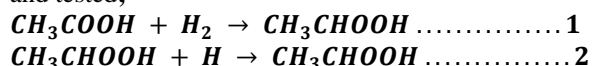


Figure 5 shows the transition state structure obtained for reaction 1. This reaction exhibits a significant barrier height (72.92 kcal/mol as shown in Table 3) in the gas/ice phase; this could make such reaction go slowly. Reaction 2 is a barrierless one of radical-radical reactions, this entails it occur simultaneously without activation barrier. A reasonably high barrier was found for reaction 3 in the gas phase. However, no transition state was found for reactions 4 and 5.

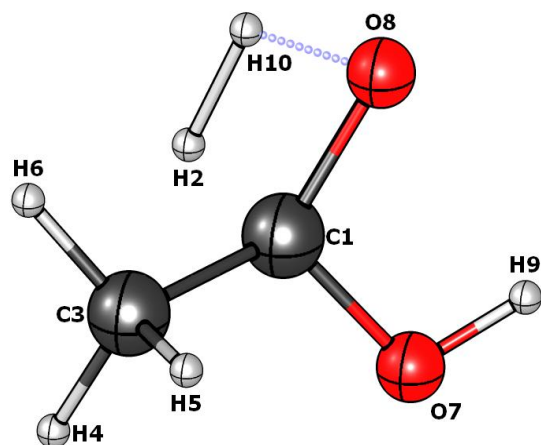


Figure 5: Transition state structure (TST) of reaction R1 (hydrogen abstraction by the oxygen and addition to the alpha carbon (C position) of acetic acid)

Table 3: Energetics of the tested reactions

Reaction number	Method	Gas phase activation barrier (Kcal/mol)
R1	B3LYP/6-31+G (d,p)	72.92
R3	B3LYP/6-31+G (d,p)	36

Destruction pathways

- (i) Using some dominant ions and neutrals in the ISM
- (ii) Photo-dissociation by direct and induced photons

Astrophysical Implications

Evidence of the presence of the various components reactants and products from the studied formation pathways have been explored to ascertain the possibility of finding 1,1-ethanediol. Acetic acid in reaction 1 has been detected in the ISM [25, 26] while hydrogen, a primary component of the ISM [27]. The reaction 1 has very high activation energy [28, 29]. This observation was extensively analysed; energy sources in the ISM in the form of shock waves (arising from the interaction of the Earth's magnetic field with the solar wind, molecular outflows during star formation, supernova blasts and galaxies colliding with each other) provide energy for both the formation and distribution of large interstellar species or those with high activation barrier, this explains the feasibility of the reaction despite the high energy barrier. The reactants species in reaction 2 are protonated acetic acid [30] and a proton, a barrierless reaction. Owing to the prevalent nature of hydrogen proton in the ISM and the acetic acid, the presence of the protonated acetic acid analogue is possible which could then react with a proton forming 1,1-ethanediol. Acetaldehyde is one of the very important molecules of Astrochemical relevance in the formation of amino acid with many works on detection and formation on ice surface [31, 32, 33]; the ubiquitous nature of water has been discussed [34]. All things being equal, ethane-1,1-diol could be found in such environments where its component species

found (both ice-phase or gas phase) in the ISM since it is possible that it could be formed in the ice mantle and/or desorption to the gas phase. Since it has not been detected yet, possible exploration in those areas could lead to its detection, photodissociation by direct and induced radiation can destroy this specie as well depending on its location [35, 36].

Conclusion

Given the stability of 1,1-ethanediol in comparison with the well-known and detected counterpart 1,2-ethanediol both from the global formula $C_2H_6O_2$, it is ironic that 1,1-ethanediol has not been detected in the ISM yet. Owing to the dearth of relevant information about this species which stands as a potential molecule of astrochemical relevance, we were motivated to characterise this specie to obtain the most stable conformer, compute the spectroscopic parameters necessary to explore this molecule such as the rotational constants, harmonic and anharmonic vibrational frequencies, centrifugal distortion constants etc, we also suggested and studied possible formation and destruction pathways and their implications in the astrophysical environments were discussed. The result shows that 1,1-ethanediol absorb within the far and medium IR window; Infrared astronomy or radioastronomical observation of this species may yield interesting outcomes due to its relatively high stability and now presence of spectroscopic parameters.

Conflict of interest: The authors declare no conflict of interest.

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