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Quantum Chemical Studies on C_2H_2O Isomeric Species: Astrophysical Implications, and Comparison of Methods

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Abstract: *The study of isomers of C_2H_2O has been the focus of numerous experimental and theoretical studies because of their significance in atmospheric chemistry, combustion processes, astrochemistry and other fields of science. ketene is a known interstellar molecular specie amongst the C_2H_2O isomeric group. In this study, we employed different computational methods gaussian-4, gaussian-3, gaussian 2, Moller-plessets-2 (G4, G3, G2 and MP2) and W2U to investigate the properties (structural and spectroscopic parameters) of all the possible isomers of the C_2H_2O isomeric group with the aim of attempting to bridge the gap between theory and experiment. We calculated the bond lengths, bond angles, vibrational frequencies, rotational constants, dipole moments and standard enthalpies of formation for each of the isomers using the various computational methods listed above. The results show that some computational methods effectively elucidate the properties of C_2H_2O isomers and provide accurate results as compared to others. The results obtained indicated that theoretical calculations are informative in the provision of explanation for several molecular properties of the isomers.*

Keywords: *Computational chemistry, Astrochemistry, Oxirene, Ethynol, Ketene*

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1.0 Introduction

In computational chemistry, mathematical phenomena are useful in predicting models that can align or be compared with experimental outcomes, thereby providing avenues for the prediction of results, whose experimental information have not been obtained (Keith *et al*., 2021) . Computational chemistry can also provide information on some descriptors that can reveals electronic structure, interaction energy and other properties of stable and unstable molecules, most of which cannot be easily derived from experimental data. This field of study allows one to understand electronic structures and models, as well as the types of interactions that molecules go through, not only for stable molecules as is typically provided by experimental procedures, but also for unstable analogues or short-lived intermediates that may be difficult to study in the lab. (Cramer, 2004; Etim *et al*., 2018a; Zöllner *et al*., 2020)

Computational chemistry has been applied in different fields of chemistry where researchers have been able to make accurate predictions of future reactions (Xiaoyue, 2022). Physicochemical properties, docking, rate constants, protein calculations, calculations of potential energy surfaces, electronic structures of molecules and their isomers, molecules in the interstellar medium (ISM) (Etim *et al*., 2017).

Compounds with the same molecular formula but different overall chemical structures are referred to as isomers (McMurry, 2008). Isomers are substances that have the same qualitative and quantitative elemental makeup; as a result, their relative molecular weights and general formulae are the same, but their structures, such as the order of their bonds and/or how they organize their atoms or groups in space, differ. Although recent developments in experimental methods have substantially aided the study of the thermochemistry and molecular structure of gas phase ions, there are still frequent issues in clearly interpreting the experimental results concerning isomers. In this regard, theoretical estimates of ion structure and stability are supporting, and in some cases directing, an experimental study in an increasingly valuable way (Etim *et al*., 2021).

Structural isomers can be used to evaluate molecular cloud chemistry models and provide information about the physical and chemical characteristics of interstellar settings (Turner *et al*., 2020). Consequently, the prediction of interstellar chemical pathways needs to be able to precisely identify the amount of complex organic molecules building components in interstellar settings. Ethynol, often referred to as hydroxy acetylene, and ketene is two potential reactants that can produce larger complex organic molecules. Both of these compounds are part of the C_2H_2O isomer family. Both the carbon–carbon double bond and the carbon–oxygen double bond exists in ketene. The triple bond between carbon atoms in ethanol is joined by a hydroxyl group (Tanaka and Yoshimine, 1980).

Arising from the lack of adequate experimental information on electronic and other properties of the stated isomers and the need to expand knowledge on the molecules, due to their usefulness, the present study is aimed at investigating the C_2H_2O system. The oxirene molecular specie is a very fascinating molecular specie. Many theoretical and experimental studies on the neutral system C_2H_2O have been done to determine if there are any more stable isomers besides ketene ($CH_2=C=O$). The isomers of C_2H_2O are a group of molecules with two carbon atoms, two hydrogen atoms and one oxygen atom, which form various structures with unique geometries and electronic configurations. These isomers are of great interest to chemists and physicists due to their importance in different fields such as astrochemistry Etim *et al*., 2016). Every observation of a molecule in the interstellar medium is more relevant because it provides meaningful information regarding the presence of potential molecules. The scientific information regarding where it was observed also serves as a reference point to which other possible molecules can be detected in the interstellar medium (Guélin and Cernicharo, 2022). Several researches have been conducted solely on the production of ketene in interstellar ice analogs. Hudson and Loeffler (2013) identified ketene in protonirradiated binary ice combinations using infrared spectroscopy. Furthermore, electron-induced chemistry with isotope-labeled reactants combined with mass spectrometry validated the synthesis of various derivatives, such as ketene and vinyl alcohol (Abplanalpa *et al*., 2016). The positive impact of the recent development and advances in astronomical and spectroscopic methods propels for a better understanding of the science (physics and chemistry) of the interstellar medium and in probing deep into the interior of the molecular clouds.

2.0 Computational Methods

In this study, the gaussian 09 software package was employed for all optimization and frequency calculations of which were carried out at the G4, G3, G2 W2U and MP2 levels of theory (Mclean and Chandler, 1980; Petersson *et al*., 1998, Curtiss, *et al*., 2007). Moller-Plesset perturbation theory (MP2) was used with the 6-31* basis set in carrying out the calculations The bond lengths, bond angles, vibrational frequencies, rotational constants, enthalpy of formation and dipole moments of the C_2H_2O isomeric groups were then calculated. Comparisons were then made to further understand, as well as bridge the gap between theoretical and experimental data. The optimized geometries were found to be stable with no imaginary frequencies

3.0 Results and Discussion

The computational studies of isomeric species gave rise to a lot of information regarding this specie. The most important of this information is the possibility of their detection in the interstellar medium. This begs the question "How can these species be detected?" The single most important information in the detection of molecules is their spectroscopic data. The spectroscopic data of every molecule differs, meaning that all molecules give off different vibrational frequencies at different intensities. The spectra emitted by a particular molecule are unique and hence, only one molecule can give off that exact frequency at that particular intensity. The various intensities observed serve as primary data to be used in the detection and confirmation of these molecules in the interstellar medium.

We compared our theoretical results with available experimental data. We found that our calculated bond lengths, bond angles, vibrational frequencies, rotational constants, dipole moments, and enthalpies were generally in good agreement with the experimental values, where available. However, there were some discrepancies between the two sets of data, particularly for the dipole moments and rotational constants of the isomers.

3.1 Enthalpy of formation

The most important aspect of the thermochemistry of C_2H_2O is the energy changes such as enthalpy of formation. The experimental measurement of heat of formation is always inaccurate due to the loss of heat to the environment (Gorai *et al*., 2017). The standard enthalpy of formation describes the feasibility of a reaction. It describes whether a reaction can take place or not (Weisenburger *et al*., 2007). The enthalpy of formation shows that ketene is the most stable isomer of C_2H_2O, having the highest enthalpy of formation, while oxirene is the least stable isomer of C_2H_2O. It has been discovered that certain molecular species with empirically verified values react favorably to predictions made using the G4 compound Model (Frisch, 2009).

The calculated enthalpies of the formation of oxirene, ketene, and ethynol were found to be in good agreement with the experimental values available in the literature, since the coefficient of determination (0.9991) was extremely close to unity.

Table 1: Enthalpy of formation of C_2H_2O isomers and their percentage errors in parenthesis

Molecules	**Enthalpy of formation d_fH^0 kcal/mol (%Error)**					
	Experimental	G4	G3	G2	W2U	MP2/6-31*
Ketene	21.25	22.316 (3.8)	22.85 (7.1)	24.34 (14.5)	23.01 (8.2)	26.56 (19.9)
Oxirene	-	66.3	65.0	67.5	68.6	69.7
Ethynol	20.43	21.980 (7.6)	22.46 (9.9)	22.84 (11.8)	22.66 (10.9)	23.14 (13.3)

3.2 Vibrational spectroscopy

The most stable isomer of the C_2H_2O isomeric group is ketene. The vibrational frequencies are shown in Tables 2-3 along with the accompanying spectrum in Figures 1-3. The results contain the vibrational frequencies and related spectra for the remaining isomers of the C_2H_2O isomeric group (Tables 2-3). The estimated and measured values of ketene and its isomers' vibrational frequencies are shown in Tables 2-4. Between 1.71 and 33.02 cm^{-1} is the range of the error between the values. The calculated values and the reported experimental values agree quite well. As a result, it is assumed that the values estimated at the G4 level are accurate for the remaining isomers that lack experimentally observed vibrational frequencies. This is due to the high coefficient of determination (0.9748) was extremely close to unity.

Several molecular species with experimentally established values have been observed to respond well to predictions made using the G4 compound method (Frisch, 2009). The vibrational spectroscopy parameters have a variety of uses, but they are particularly helpful for astronomical observations of interstellar molecular species without a dipole moment (Etim and Arunan, 2016).

Table 2: Vibrational frequencies and IR intensities of C_2H_2O isomers

Ketene		**Oxirene**		**Ethynol**	
Frequency (cm^{-1})	**Intensity**	**Frequency (cm^{-1})**	**Intensity**	**Frequency (cm^{-1})**	**Intensity**
450.29	2.7515	328.75	23.5537	491.70	9.7907
552.87	100.9396	579.37	133.0011	622.21	32.9639
594.20	17.7055	754.89	119.2105	723.87	159.5372
993.02	5.5189	1027.21	4.0752	1112.09	11.2480
1177.18	6.2108	1181.10	18.5166	1266.22	4.6959
1414.70	15.8288	1454.71	20.0735	1566.87	14.9723
2246.59	528.2304	1546.20	47.9977	2377.98	917.4536
3194.61	26.0727	3096.41	36.5587	3376.57	23.3398
3289.12	7.9046	3156.13	1.6812	3477.25	3.6379

Table 3: Vibrational frequencies of ketene

Calculated Frequency (Cm^{-1})	**Experimental frequency (Cm^{-1})**	**Percentage error (%)**
450.29	454	0.89
552.87	550	0.52
594.20	592	0.37
993.02	960	3.32
1177.18	1189	1.02
1414.70	1391	1.63
2246.59	2363	0.76
3194.61	3209	0.47
3289.12	3286	0.09

3.3 Rotational constants

Rotational spectroscopy remains a very important spectroscopic Parameter employed in the astronomical observation of molecular species from different regions of the interstellar medium. The experimentally measured rotational constants (from the NIST Webbook) for ketene and its isomers are presented in Table 3. The calculated rotational constants show great similarity to the experimentally obtained rotational constants, having little error. Although the results obtained using the MP2/6-31* computational method produced the least accurate result for all rotational constants, A, B and C. Thereby having percentage errors ranging from 2.4 – 4.2%. The very low errors were also backed up by the very high coefficient of determination (0.9871).

Table 4: Rotational constants of C_2H_2O isomers and their corresponding percentage error with respect to the experimental data in parenthesis

Molecular specie		**Rotational Constants (GHZ)**		
		A	B	C
Ketene	Experimental	280.906	10.293	9.915
	Calculated using G4	284.10 (1.13)	10.08 (2.1)	9.735 (1.92)
	Calculated using G3	284.1 (1.13)	10.08 (2.1)	9.735 (1.8)
	Calculated using G2	284.09(1.14)	10.080 (2.1)	9.735 (1.8)
	Calculated using W2U	284.09 (1.14)	10.081 (2.1)	9.735 (1.8)
	Calculated using MP2/6-31*	272.3(4.2)	9.998 (2.9)	9.673 (2.4)
Oxirene	Calculated using G4	33.005	25.857	14.498
	Calculated using G3	33.005	25.857	14.498
	Calculated using G2	34.769	26.997	15.197
	Calculated using W2U	33.005	25.857	14.498
	Calculated using MP2/6-31*	34.18	29.03	15.70
Ethynol	Calculated using G4	667.139	9.78456	9.64313
	Calculated using G3	667.14	9.7846	9.6431
	Calculated using G2	667.14	9.7846	9.6431
	Calculated using W2U	684.38	9.7816	9.6437
	Calculated using MP2/6-31*	585.5	9.496	9.349

3.4 Structural parameters

The bond lengths and bond angles of Ketene and its isomers are presented in Table 5, while Fig. 1 depicts the optimized geometry. As shown in the Table, there is an excellent agreement between the experimentally measured values and the computationally predicted values. For example, both the experimental (1.314Å) and the computational (1.308Å) values for C7-C bond length were extremely similar. For the other bond lengths reported for ketene and its isomers, the difference between the experimental and the computational values range between 0.001-0.2 Å, hence proving that the G4 method is the most accurate method amongst the computational methods of interest. While for the predicted bond angles, the difference between the experimental and the computational values was discovered to be nearly infinitesimal. Some molecular species with empirically validated values have been shown to respond positively to predictions provided using the G4 compound Model (Frisch, 2009). These findings suggest that the bond lengths and bond angles predicted with the G4 method can stand for the other isomers of the C_2H_2O isomeric group which have no experimental data on the structural parameters of the C_2H_2O presented in Table 5.

The bond angles also show that the G4 method is extremely accurate since the percentage error ranges from 0.00-1.67. The bond lengths and bond angles showed great coherence between the theoretical and experimental values by having coefficients of determination of 0.9982 and 0.9917 respectively.

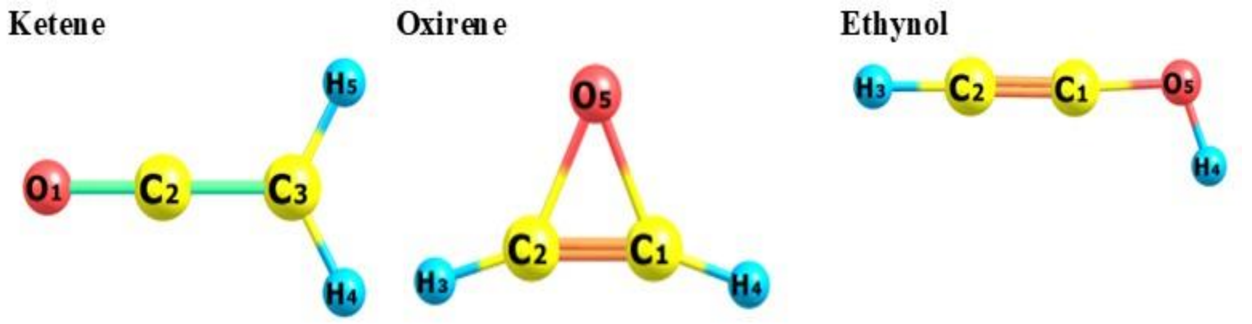

Fig. 1: Optimized geometry for ketene, oxirene and ethynol

Table 5: Bond lengths (Å) and bond angles $(^0)$ of C_2H_2O isomers

	Ketene			**Oxirene**		**Ethynol**
Parameters	Calculated	Experimental	Parameters	Calculated	Parameters	Calculated
R(1-2)	1.163	1.162	R(1-2)	1.263	R(1-2)	1.199
R(2-3)	1.308	1.314	R(1-4)	1.071	R(1-5)	1.308
R(3-4)	1.080	1.083	R(1-5)	1.488	R(2-3)	1.060
R(3-5)	1.080	1.083	R(2-3)	1.070	R(4-5)	0.966
A(1-2-3)	180.0	180.0	A(2-1-4)	161.0	A(2-1-5)	176.4
A(2-3-4)	119.7	118.7	A(2-1-5)	66.0	A(1-2-3)	179.4
A(2-3-5)	119.7	118.7	A(1-2-3)	162.9	A(1-5-4)	110.0
A(4-3-5)	120.6	122.56	A(4-1-5)	132.9	R(1-2)	1.199

3.5 Dipole moments

The dipole moment is useful in determining the polar nature of the chemical bonds. It is also useful in astrophysics and related areas such as astrochemistry and astrobiology as the dipole of a molecule plays an important role in the astronomical observation of such molecule (Etim *et al*., 2018). The dipole moments obtained at the G4 level for all the isomeric molecular species in this study are presented in Table 7. The dipole moments of the isomers were found to vary considerably, ranging from 1.492 D for the CH_2CO isomer to 2.367 D for the oxirene isomer.

Table 5: Bond lengths (Å) and bond angles $(^0)$ of ketene

Parameters	Calculated Value	Experimental value	%
R(1-2)	1.163	1.162	0.09
R(2-3)	1.308	1.314	0.46
R(3-4)	1.080	1.083	0.28
R(3-5)	1.080	1.083	0.28
A(1-2-3)	180.0	180.0	0.00
A(2-3-4)	119.7	118.7	0.84
A(2-3-5)	119.7	118.7	0.84
A(4-3-5)	120.6	122.56	1.67

The dipole moments obtained using the G4 method elucidated the most accurate results concerning their experimental dipole moments. It has been demonstrated that several molecular species with empirically verified values react favorably to predictions made using the G4 compound Model (Frisch, 2009). The dipole moments of C_2H_2O isomers can be seen in Table 7 below.

Table 7: Dipole moments of C_2H_2O isomers and their corresponding error with respect to the experimental data

Molecule	Calculated Dipole moment (Debye) (error)					Experimental dipole moment (Debye)
	G4	W2U	MP2/6-31*	G3	G2	
Ketene	1.49 (0.07)	1.679 (0.26)	1.769 (0.35)	1.841 (0.42)	1.841 (0.42)	1.420
Oxirene	2.367	1.615	1.767	1.932	1.933	-
Ethynol	1.685	2.447	2.669	2.964	2.811	-

We compared our theoretical results with available experimental data. We found that our calculated bond lengths, bond angles, vibrational frequencies, rotational constants, dipole moments, and enthalpies were generally in good agreement with experimental values, where available.

4.0 Conclusion

In conclusion, we have investigated the properties of all the possible isomers of C_2H_2O isomeric group using different computational methods. Our calculations reveal that the properties of these isomers vary significantly depending on their structure. Our comparison with experimental data indicates that the G4 compound method provides accurate results with the experimentally obtained data. The calculations provided reliable predictions of the properties of C_2H_2O isomers. The present study describes the stability and electronic properties of C_2H_2O isomers, which could aid in the design of new materials and catalysts. The results indicate that ketene is the most stable isomer, followed by ethynol and vinyl oxirene. The results obtained using the G4 compound method could be used for the successful astronomical searches for the Ehynone and the ethynol molecular species in the interstellar medium. Because these molecular species are believed to be present in the interstellar medium.

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E.E. Etim and J.P. Shinggu conceived the idea, performed the calculations and wrote the manuscript. A.I. Onen read through the manuscript and made input in the work..

SUPPORTING INFORMATION

Table A1: Bond lengths (Å), bond angles (Degrees ^{0}) and vibrational frequencies (cm^{-1}) of C_2H_2O isomers using MP2/6-31*

	Ketene		Oxirene		Ethynol
Parameters		Parameters		Parameters	
R(1-2)	1.181	R(1-2)	1.277	R(1-2)	1.216
R(2-3)	1.320	R(1-4)	1.074	R(1-5)	1.326
R(3-4)	1.080	R(1-5)	1.502	R(2-3)	1.064
R(3-5)	1.080	R(2-3)	1.073	R(4-5)	0.975
A(1-2-3)	180.0	A(2-1-4)	161.1	A(2-1-5)	176.7
A(2-3-4)	119.6	A(2-1-5)	65.9	A(1-2-3)	179.1
A(2-3-5)	119.6	A(1-2-3)	162.7	A(1-5-4)	108.8
A(4-3-5)	120.8	A(4-1-5)	133.1	W1(A)	283.6
W1(A)	437.5	W1(A)	-33.2	W2(A)	313.4
W2(A)	516.3	W2(A)	446.1	W3(A)	507.5
W3(A)	582.6	W3(A)	500.5	W4(A)	561.1
W4(A)	1019.3	W4(A)	888.0	W5(A)	1075.6
W5(A)	1172.9	W5(A)	950.5	W6(A)	1284.7
W6(A)	1451.6	W6(A)	1108.6	W7(A)	2253.9
W7(A)	2235.1	W7(A)	1799.5	W8(A)	3549.5
W8(A)	3266.6	W8(A)	3389.5	W9(A)	3738.1
W9(A)	3370.9	W9(A)	3458.3	R(1-2)	1.216

Table A2: Bond lengths (Å), bond angles (Degrees ^{0}) and vibrational frequencies (cm^{-1}) of C_2H_2O isomers using G4

	Ketene		Oxirene		Ethynol
Parameters	G4	Parameters	G4	Parameters	G4
R(1-2)	1.163	R(1-2)	1.263	R(1-2)	1.199
R(2-3)	1.308	R(1-4)	1.071	R(1-5)	1.308
R(3-4)	1.080	R(1-5)	1.488	R(2-3)	1.060
R(3-5)	1.080	R(2-3)	1.070	R(4-5)	0.966
A(1-2-3)	180.0	A(2-1-4)	161.0	A(2-1-5)	176.4
A(2-3-4)	119.7	A(2-1-5)	66.0	A(1-2-3)	179.4
A(2-3-5)	119.7	A(1-2-3)	162.9	A(1-5-4)	110.0
A(4-3-5)	120.6	A(4-1-5)	132.9	W1(A)	398.0
W1(A)	450.3	W1(A)	-170.9	W2(A)	410.1
W2(A)	552.9	W2(A)	538.6	W3(A)	526.6
W3(A)	594.2	W3(A)	591.9	W4(A)	619.7
W4(A)	993.0	W4(A)	894.6	W5(A)	1092.2
W5(A)	1177.2	W5(A)	948.8	W6(A)	1254.4
W6(A)	1414.7	W6(A)	1083.2	W7(A)	2311.4
W7(A)	2246.6	W7(A)	1836.2	W8(A)	3517.4
W8(A)	3194.6	W8(A)	3338.9	W9(A)	3775.9
W9(A)	3289.1	W9(A)	3415.5	R(1-2)	1.199

Table A3: Bond lengths (Å), bond angles (Degrees ^{0}) and vibrational frequencies (cm^{-1}) of C_2H_2O isomers using G2

	Ketene		**Oxirene**		**Ethynol**
Parameters	G2	Parameters	G2	Parameters	G2
R(1-2)	1.145	R(1-2)	1.244	R(1-2)	1.183
R(2-3)	1.306	R(1-4)	1.062	R(1-5)	1.304
R(3-4)	1.071	R(1-5)	1.467	R(2-3)	1.055
R(3-5)	1.071	R(2-3)	1.062	R(4-5)	0.950
A(1-2-3)	180.0	A(2-1-4)	162.7	A(2-1-5)	178.5
A(2-3-4)	119.3	A(2-1-5)	64.9	A(1-2-3)	179.8
A(2-3-5)	119.3	A(1-2-3)	162.8	A(1-5-4)	110.4
A(4-3-5)	121.3	A(4-1-5)	132.3	W1(A)	463.5
W1(A)	491.7	W1(A)	439.6	W2(A)	532.7
W2(A)	622.2	W2(A)	693.4	W3(A)	700.1
W3(A)	723.9	W3(A)	795.6	W4(A)	796.8
W4(A)	1112.1	W4(A)	997.7	W5(A)	1168.3
W5(A)	1266.2	W5(A)	1094.9	W6(A)	1385.7
W6(A)	1566.9	W6(A)	1180.2	W7(A)	2480.7
W7(A)	2378.0	W7(A)	2004.5	W8(A)	3683.2
W8(A)	3376.6	W8(A)	3536.9	W9(A)	4066.0
W9(A)	3477.2	W9(A)	3618.1	R(1-2)	1.183

Table A4: Bond lengths (Å), bond angles (Degrees ^{0}) and vibrational frequencies (cm^{-1}) of C_2H_2O isomers using G3

	Ketene		**Oxirene**		**Ethynol**
Parameters	G3	Parameters	G3	Parameters	G3
R(1-2)	1.145	R(1-2)	1.244	R(1-2)	1.183
R(2-3)	1.306	R(1-4)	1.062	R(1-5)	1.304
R(3-4)	1.071	R(1-5)	1.467	R(2-3)	1.055
R(3-5)	1.071	R(2-3)	1.062	R(4-5)	0.950
A(1-2-3)	180.0	A(2-1-4)	162.7	A(2-1-5)	178.5
A(2-3-4)	119.3	A(2-1-5)	64.9	A(1-2-3)	179.8
A(2-3-5)	119.3	A(1-2-3)	162.8	A(1-5-4)	110.4
A(4-3-5)	121.3	A(4-1-5)	132.3	W1(A)	463.5
W1(A)	491.7	W1(A)	439.6	W2(A)	532.7
W2(A)	622.2	W2(A)	693.4	W3(A)	700.1
W3(A)	723.9	W3(A)	795.6	W4(A)	796.8
W4(A)	1112.1	W4(A)	997.7	W5(A)	1168.3
W5(A)	1266.2	W5(A)	1094.9	W6(A)	1385.7
W6(A)	1566.9	W6(A)	1180.2	W7(A)	2480.7
W7(A)	2378.0	W7(A)	2004.5	W8(A)	3683.2
W8(A)	3376.6	W8(A)	3536.9	W9(A)	4066.0
W9(A)	3477.2	W9(A)	3618.1	R(1-2)	1.183

Table A5: Bond lengths (Å), bond angles (Degrees ^{0}) and vibrational frequencies (cm^{-1}) of C$_2$H$_2$O isomers using W2U

	Ketene		Oxirene		Ethynol
Parameter	W2U	Parameter	W2U	Parameter	W2U
R(1-2)	1.158	R(1-2)	1.259	R(1-2)	1.196
R(2-3)	1.308	R(1-4)	1.069	R(1-4)	1.307
R(3-4)	1.078	R(1-5)	1.486	R(2-5)	1.059
R(3-5)	1.077	R(2-3)	1.068	R(3-4)	0.964
A(1-2-3)	180.0	A(2-1-4)	160.9	A(2-1-4)	176.2
A(2-3-4)	119.6	A(2-1-5)	66.0	A(1-2-5)	179.5
A(2-3-5)	119.6	A(1-2-3)	162.7	A(1-4-3)	110.7
A(4-3-5)	120.8	A(4-1-5)	133.0	W1(A)	396.8
W1(A)	437.5	W1(A)	-151.0	W2(A)	437.7
W2(A)	548.6	W2(A)	542.2	W3(A)	544.9
W3(A)	589.1	W3(A)	661.2	W4(A)	649.2
W4(A)	989.9	W4(A)	889.0	W5(A)	1088.7
W5(A)	1173.5	W5(A)	967.8	W6(A)	1250.3
W6(A)	1412.9	W6(A)	1068.7	W7(A)	2289.4
W7(A)	2232.3	W7(A)	1834.7	W8(A)	3491.0
W8(A)	3185.2	W8(A)	3325.3	W9(A)	3782.7
W9(A)	3277.6	W9(A)	3400.5	R(1-2)	1.196

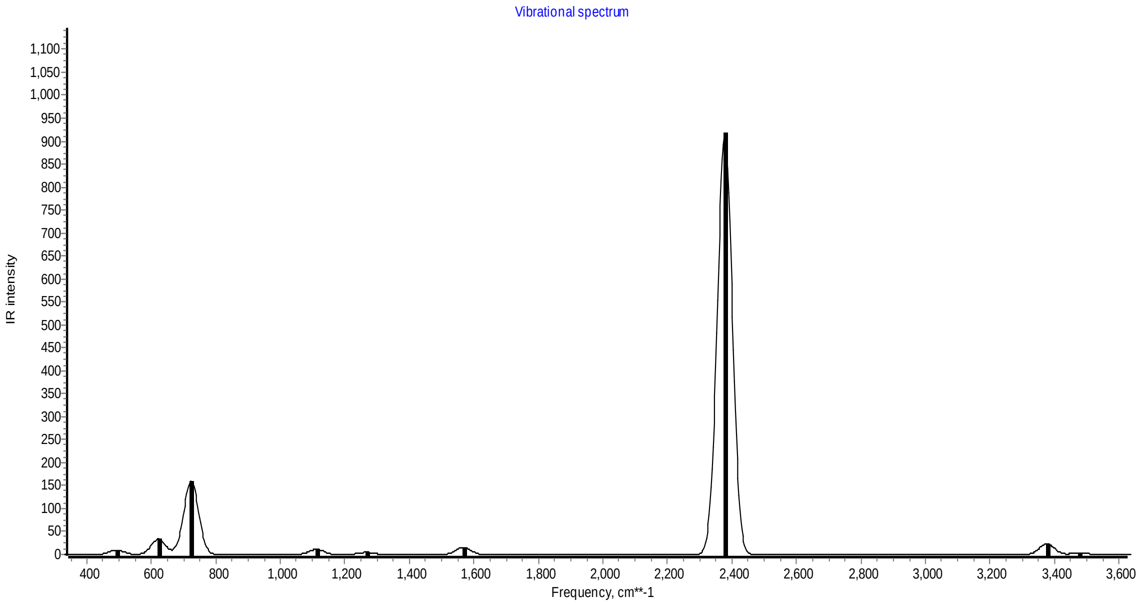

Fig. 1: Calculated IR Intensities for ketene

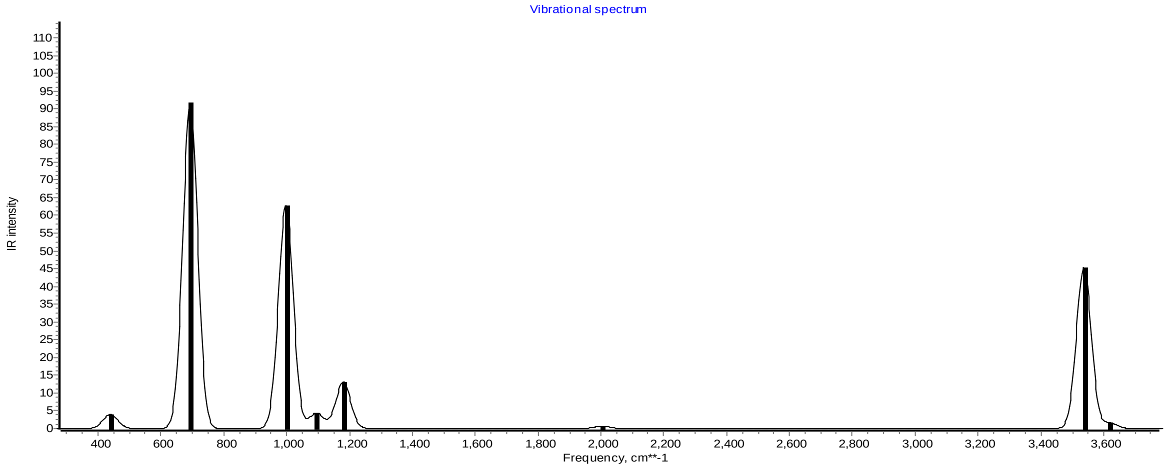

Fig. 2 : Calculated IR Intensities for Oxirene

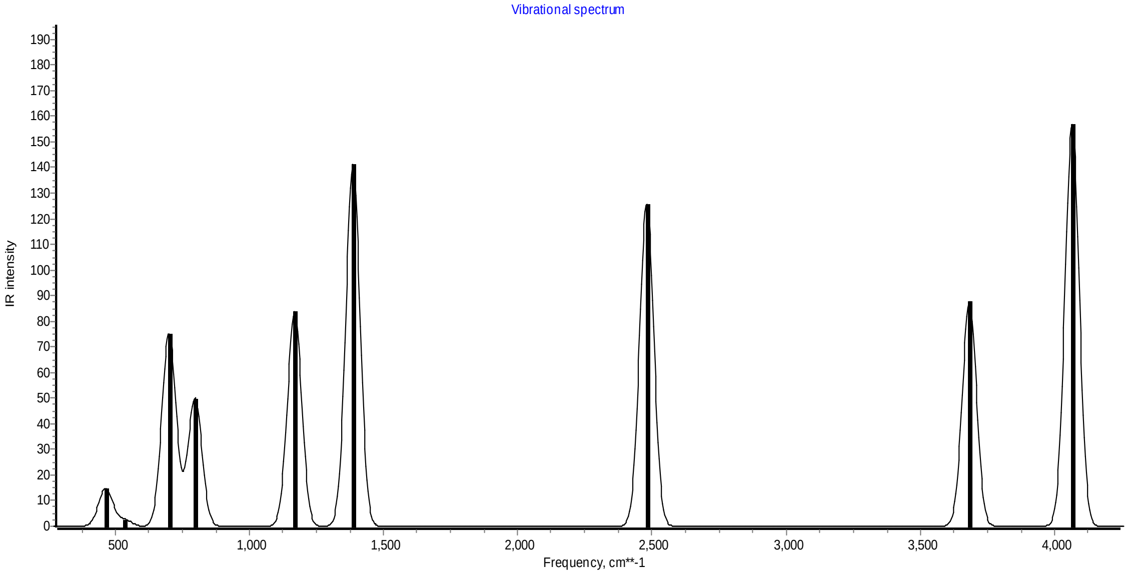

Fig. 3 : Calculated IR Intensities for Ethynol