



Supporting Information

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Supporting Information for:

The Lowest Singlet and Triplet States of the Oxyallyl Diradical

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This Supporting Information provides a brief description of the electronic structure methods employed in the present study. The results of the calculations follow the description. Optimized geometries, energies, harmonic vibrational frequencies, and thermal corrections for the molecules relevant to this study are tabulated.

Calculations were carried out using the Gaussian 03¹ and Molcas². Geometry optimizations were performed using (U)B3LYP³ and complete active space self-consistent-field (CASSCF) calculations with (4/4) active space.⁴ In the case of oxyallyl, the CAS consists of all configurations that come from placing four electrons in four π molecular orbitals. For consistency, four electrons were also correlated in four orbitals for the cyclopropanones using the π and π^* orbitals of the carbonyl bond and the σ and σ^* orbitals of the C2-C3 bond. The orbitals chosen for the transition state are naturally the ones that correlate with those chosen for cyclopropanone and oxyallyl which give the lowest CASSCF energies. The calculations were performed with the 6-311++G(d,p)⁵ and cc-pVTZ basis sets.⁶ The latter was augmented by diffuse functions⁷ in some calculations. To include the effects of dynamic electron correlation,⁸ single-point CASPT2 calculations⁹ were carried out at each (4/4)CASSCF stationary point.

	1A_1	3B_2	1A_1	TS-ring-closure
(U)B3LYP/cc-pVTZ	0	28.45	28.99	30.27
S^2 ((U)B3LYP)	0	2.028	0.805	0.510
CASSCF(4/4)/cc-pVTZ	0	21.33	24.84	24.92
CASPT2(4/4)/cc-pVTZ //CASSCF(4/4)/cc-pVTZ	0	33.12	32.72	31.96
Reference Weight	0.8425	0.8458	0.8430	0.8424

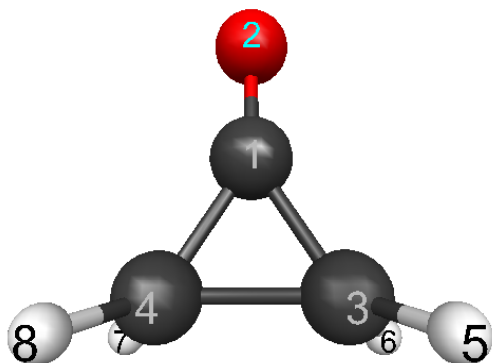
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Cyclopropanone, b3lyp/6-311++G(d,p), C_{2v} Geometry

Nuclear repulsion energy	108.772187 Hartree
Zero-point correction	0.060547 Hartree
Thermal correction to Energy	0.064569 Hartree
Thermal correction to Enthalpy	0.065513 Hartree
Thermal correction to Gibbs Free Energy	0.035328 Hartree
B3LYP/cc-PVTZ energy	-191.940607 Hartree



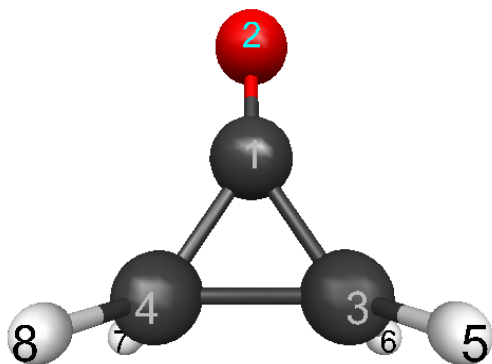
	X	Y	Z
C1	0.000000	0.000000	0.382200
O2	0.000000	0.000000	1.578960
C3	0.000000	0.787823	-0.857437
C4	0.000000	-0.787823	-0.857437
H5	0.913924	1.290098	-1.158910
H6	-0.913924	1.290098	-1.158910
H7	-0.913924	-1.290098	-1.158910
H8	0.913924	-1.290098	-1.158910

(1-2)	1.197	(1-3)	1.469	(3-4)	1.576	(3-5)	1.086
(2-1-3)	147.6	(3-1-4)	64.9	(1-3-4)	57.6	(1-3-5)	118.9
(4-3-5)	117.6	(5-3-6)	114.7				
(2-1-3-4)	180.0	(2-1-3-5)	74.0	(4-1-3-5)	-106.0		
(1-3-4-7)	108.3	(5-3-4-7)	-143.5	(5-3-4-8)	0.0		

Frequencies (cm⁻¹): 303.8 506.1 642.3 703.5 716.3 951.3 1006.6 1052.9
1061.3 1103.7 1157.9 1413.9 1432.0 1928.2 3106.5 3107.2 3185.4 3198.2

Cyclopropanone, b3lyp/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	108.981008 Hartree
Zero-point correction	0.060654 Hartree
Thermal correction to Energy	0.064667 Hartree
Thermal correction to Enthalpy	0.065611 Hartree
Thermal correction to Gibbs Free Energy	0.035448 Hartree
B3LYP/cc-PVTZ energy	-191.955807 Hartree



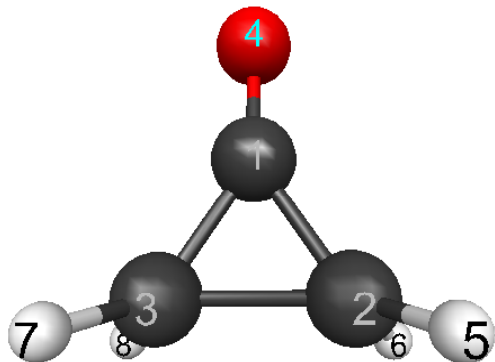
	X	Y	Z
C1	0.000000	0.000000	0.382049
O2	0.000000	0.000000	1.576571
C3	0.000000	0.785547	-0.856341
C4	0.000000	-0.785547	-0.856341
H5	0.911547	1.287260	-1.157193
H6	-0.911547	1.287260	-1.157193
H7	-0.911547	-1.287260	-1.157193
H8	0.911547	-1.287260	-1.157193

(1-2)	1.195	(1-3)	1.467	(3-4)	1.571	(3-5)	1.083
(2-1-3)	147.6	(3-1-4)	64.8	(1-3-4)	57.6	(1-3-5)	118.9
(4-3-5)	117.6	(5-3-6)	114.6				
(2-1-3-4)	180.0	(2-1-3-5)	73.9	(4-1-3-5)	-106.1		
(1-3-4-7)	108.3	(5-3-4-7)	-143.5	(5-3-4-8)	0.0		

Frequencies (cm⁻¹): 308.7 507.9 639.0 702.9 719.2 952.7 1011.8 1052.2
1065.4 1104.7 1163.4 1419.0 1434.1 1932.1 3111.3 3111.8 3187.5 3200.3

Cyclopropanone, casscf(4/4)/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	109.355156	Hartree
Zero-point correction	0.064238	Hartree
Thermal correction to Enthalpy	0.069037	Hartree
Thermal correction to Gibbs Free Energy	0.039116	Hartree
Casscf(4/4)/cc-PVTZ energy	-190.845916	Hartree
Caspt2(4/4)/cc-PVTZ//casscf(4/4)-cc-PVTZ energy	-191.508367	Hartree



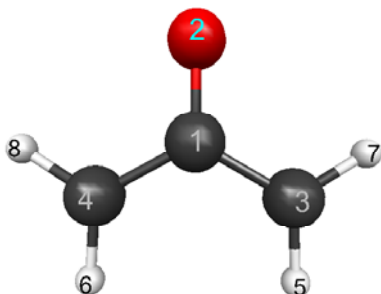
	X	Y	Z
C1	0.000000	0.000000	0.366895
C2	0.000000	0.799883	-0.852479
C3	0.000000	-0.799883	-0.852479
O4	0.000000	0.000000	1.553472
H5	0.907936	1.292139	-1.149562
H6	-0.907936	1.292139	-1.149562
H7	0.907936	-1.292139	-1.149562
H8	-0.907936	-1.292139	-1.149562

(1-2)	1.458	(1-4)	1.187	(2-3)	1.600	(2-5)	1.075
(2-1-3)	66.5	(2-1-4)	146.7	(1-2-3)	56.7	(1-2-5)	118.8
(3-2-5)	117.3	(5-2-6)	115.3				
(3-1-2-5)	-105.3	(4-1-2-3)	180.0	(4-1-2-5)	74.7		
(1-2-3-7)	-108.1	(5-2-3-7)	0.0	(5-2-3-8)	-143.8		

Frequencies (cm^{-1}): 333.9 545.9 703.7 725.8 747.0 1058.3 1073.4 1119.3
 1164.8 1183.3 1206.7 1542.1 1562.5 2036.3 3252.7 3257.1 3336.9 3348.9

Oxyallyl-³B₂, b3lyp/6-311++G(d,p), C_{2v} Geometry

Nuclear repulsion energy	104.598611 Hartree
Zero-point correction	0.056852 Hartree
Thermal correction to Energy	0.061506 Hartree
Thermal correction to Enthalpy	0.062451 Hartree
Thermal correction to Gibbs Free Energy	0.030082 Hartree
B3LYP/cc-PVTZ energy	-191.895910 Hartree
S ²	2.0276



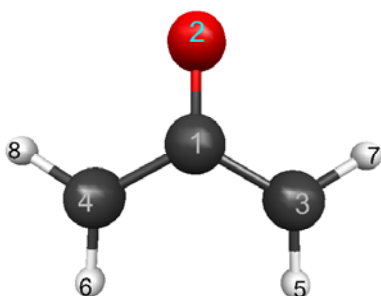
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C1	0.000000	0.000000	0.067054
O2	0.000000	0.000000	1.335228
C3	0.000000	1.254691	-0.629984
C4	0.000000	-1.254691	-0.629984
H5	0.000000	1.313048	-1.711690
H6	0.000000	-1.313048	-1.711690
H7	0.000000	2.168094	-0.050481
H8	0.000000	-2.168094	-0.050481

(1-2)	1.268	(1-3)	1.435	(3-5)	1.083	(3-7)	1.082
(2-1-3)	119.1	(3-1-4)	121.9	(1-3-5)	122.1	(1-3-7)	118.6
(5-3-7)	119.3						
(2-1-3-5)	180.0	(2-1-3-7)		0.0	(4-1-3-5)		0.0
(4-1-3-7)	180.0						

Frequencies (cm⁻¹): 269.3 408.5 420.4 520.9 540.9 682.7 779.4 900.3
935.8 1052.1 1317.5 1369.7 1465.1 1472.1 3145.2 3150.9 3261.0 3263.5

Oxyallyl-³B₂, b3lyp/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	104.822853 Hartree
Zero-point correction	0.056998 Hartree
Thermal correction to Energy	0.061628 Hartree
Thermal correction to Enthalpy	0.062573 Hartree
Thermal correction to Gibbs Free Energy	0.030252 Hartree
B3LYP/cc-PVTZ energy	-191.910469 Hartree
S ²	2.0279



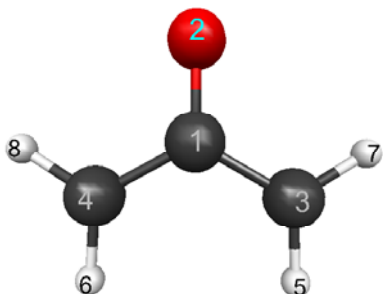
	X	Y	Z
C1	0.000000	0.000000	0.066442
O2	0.000000	0.000000	1.332357
C3	0.000000	1.252070	-0.628921
C4	0.000000	-1.252070	-0.628921
H5	0.000000	1.311519	-1.708043
H6	0.000000	-1.311519	-1.708043
H7	0.000000	2.161034	-0.047182
H8	0.000000	-2.161034	-0.047182

(1-2)	1.266	(1-3)	1.432	(3-5)	1.081	(3-7)	1.079
(2-1-3)	119.0	(3-1-4)	121.9	(1-3-5)	122.2	(1-3-7)	118.3
(5-3-7)	119.5						
(2-1-3-5)	180.0	(2-1-3-7)		0.0	(4-1-3-5)		0.0
(4-1-3-7)	180.0						

Frequencies (cm⁻¹): 275.8 407.4 428.6 521.2 539.9 693.4 788.8 899.9
938.2 1056.5 1318.6 1375.1 1468.7 1475.3 3148.7 3154.4 3263.1 3265.5

Oxyallyl-³B₂, b3lyp/aug-cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	104.803384 Hartree
Zero-point correction	0.057003 Hartree
Thermal correction to Energy	0.061635 Hartree
Thermal correction to Enthalpy	0.062579 Hartree
Thermal correction to Gibbs Free Energy	0.030253 Hartree
B3LYP/cc-PVTZ energy	-191.913699 Hartree
S ²	2.0275



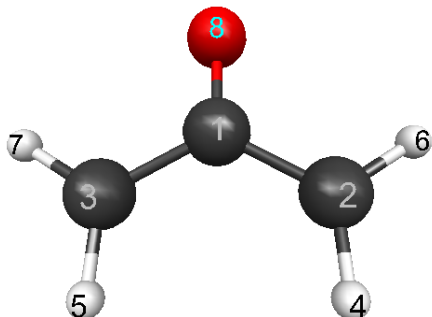
	X	Y	Z
C1	0.000000	0.000000	0.066417
O2	0.000000	0.000000	1.332929
C3	0.000000	1.252251	-0.628840
C4	0.000000	-1.252251	-0.628840
H5	0.000000	1.309195	-1.707948
H6	0.000000	-1.309195	-1.707948
H7	0.000000	2.162929	-0.049980
H8	0.000000	-2.162929	-0.049980

(1-2)	1.267	(1-3)	1.432	(3-5)	1.081	(3-7)	1.079
(2-1-3)	119.0	(3-1-4)	121.9	(1-3-5)	122.1	(1-3-7)	118.5
(5-3-7)	119.4						
(2-1-3-5)	180.0	(2-1-3-7)		0.0	(4-1-3-5)		0.0
(4-1-3-7)	180.0						

Frequencies (cm⁻¹): 274.2 408.1 425.1 520.8 540.1 698.3 792.3 900.0
938.7 1055.7 1319.2 1372.5 1470.1 1475.5 3149.2 3154.9 3262.0 3264.5

Oxyallyl-³B₂, casscf(4/4)/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	105.311927 Hartree
Zero-point correction	0.059696 Hartree
Thermal correction to Enthalpy	0.065123 Hartree
Thermal correction to Gibbs Free Energy	0.034144 Hartree
Casscf(4/4)/cc-PVTZ energy	-190.811930 Hartree
Caspt2(4/4)/cc-PVTZ//casscf(4/4)/cc-PVTZ energy	-191.455589 Hartree



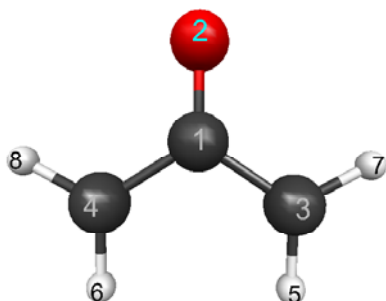
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C1	0.000000	0.000000	0.051553
C2	0.000000	1.254650	-0.654194
C3	0.000000	-1.254650	-0.654194
H4	0.000000	1.298704	-1.724112
H5	0.000000	-1.298704	-1.724112
H6	0.000000	2.163404	-0.089296
H7	0.000000	-2.163404	-0.089296
O8	0.000000	0.000000	1.292858

(1-2)	1.440	(1-8)	1.241	(2-4)	1.071	(2-6)	1.070
(2-1-3)	121.3	(2-1-8)	119.4	(1-2-4)	121.7	(1-2-6)	118.8
(4-2-6)	119.5						
(3-1-2-4)	0.0	(3-1-2-6)		180.0	(8-1-2-4)		180.0
(8-1-2-6)	0.0						

Frequencies (cm⁻¹): 380.5 430.3 444.1 550.0 558.2 604.8 701.2 913.2
1007.7 1139.5 1389.6 1460.0 1586.7 1589.4 3302.6 3307.9 3415.9 3419.1

Oxyallyl-¹A₁, b3lyp/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	104.967566 Hartree
Zero-point correction	0.057172 Hartree
Thermal correction to Energy	0.062000 Hartree
Thermal correction to Enthalpy	0.062945 Hartree
Thermal correction to Gibbs Free Energy	0.031126 Hartree
B3LYP/cc-PVTZ energy	-191.909601 Hartree
S ²	0.8048



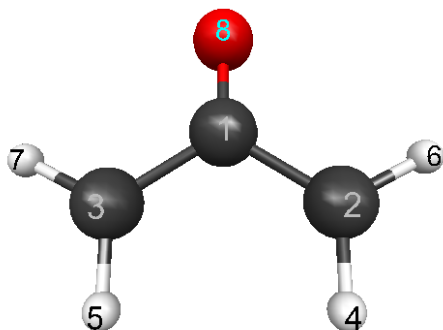
	X	Y	Z
C1	0.000000	0.000000	0.125659
O2	0.000000	0.000000	1.360443
C3	0.000000	1.218751	-0.656275
C4	0.000000	-1.218751	-0.656275
H5	0.000000	1.203671	-1.736940
H6	0.000000	-1.203671	-1.736940
H7	0.000000	2.170691	-0.144163
H8	0.000000	-2.170691	-0.144163

(1-2)	1.235	(1-3)	1.448	(3-5)	1.081	(3-7)	1.081
(2-1-3)	122.7	(3-1-4)	114.6	(1-3-5)	121.9	(1-3-7)	119.0
(5-3-7)	119.1						
(2-1-3-5)	180.0	(2-1-3-7)	0.0	(4-1-3-5)	0.0		
(4-1-3-7)	180.0						

Frequencies (cm⁻¹): 154.9 388.6 459.5 478.3 495.5 794.4 824.8 884.4
910.9 1059.9 1269.3 1465.1 1470.4 1632.5 3142.0 3148.4 3256.5 3260.1

Oxyallyl-¹A₁, casscf(4/4)/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	104.967566 Hartree
Zero-point correction	0.057172 Hartree
Thermal correction to Enthalpy	0.062945 Hartree
Thermal correction to Gibbs Free Energy	0.031126 Hartree
Casscf(4/4)/cc-PVTZ energy	-190.806330 Hartree
Caspt2(4/4)/cc-PVTZ//casscf(4/4)/cc-PVTZ energy	-191.456222 Hartree



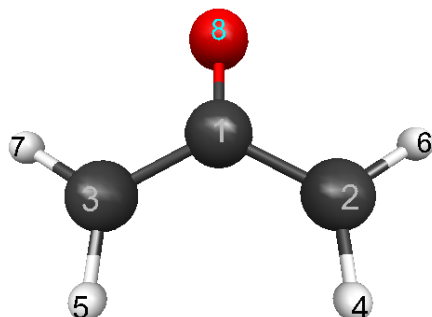
	X	Y	Z
C1	0.000000	0.000000	0.144722
C2	0.000000	1.223571	-0.655522
C3	0.000000	-1.223571	-0.655522
H4	0.000000	1.186576	-1.724920
H5	0.000000	-1.186576	-1.724920
H6	0.000000	2.174860	-0.162772
H7	0.000000	-2.174860	-0.162772
O8	0.000000	0.000000	1.350914

(1-2)	1.462	(1-8)	1.206	(2-4)	1.070	(2-6)	1.071
(2-1-3)	113.6	(2-1-8)	123.2	(1-2-4)	121.2	(1-2-6)	119.4
(4-2-6)	119.4						
(3-1-2-4)	0.0	(3-1-2-6)	180.0	(8-1-2-4)	180.0		
(8-1-2-6)	0.0						

Frequencies (cm⁻¹): 88.2 405.8 442.4 532.6 538.8 707.0 733.8 904.8
984.4 1146.3 1362.0 1584.5 1588.7 1875.6 3301.9 3307.9 3417.3 3422.7

Oxyallyl- 1A_1 , casscf(4/4)/aug-cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	105.389436 Hartree
Zero-point correction	0.064269 Hartree
Thermal correction to Enthalpy	0.069003 Hartree
Thermal correction to Gibbs Free Energy	0.039054 Hartree
Casscf(4/4)/aug-cc-PVTZ energy	-190.809643 Hartree
Caspt2(4/4)/aug-cc-PVTZ//casscf(4/4)/aug-cc-PVTZ energy	-191.473705 Hartree



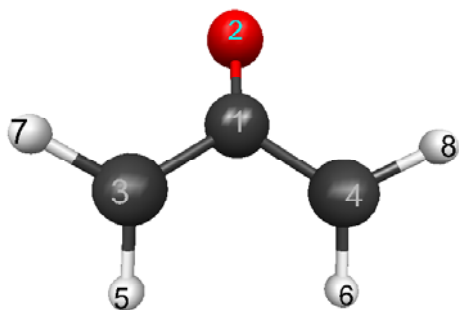
	X	Y	Z
C1	0.000000	0.000000	0.144805
C2	0.000000	1.222074	-0.655125
C3	0.000000	-1.222074	-0.655125
H4	0.000000	1.183130	-1.724424
H5	0.000000	-1.183130	-1.724424
H6	0.000000	2.174404	-0.164303
H7	0.000000	-2.174404	-0.164303
O8	0.000000	0.000000	1.352106

(1-2)	1.461	(1-8)	1.207	(2-4)	1.070	(2-6)	1.071		
(2-1-3)	113.6	(2-1-8)	123.2	(1-2-4)	121.1	(1-2-6)	119.5		
(4-2-6)	119.4								
(3-1-2-4)		0.0	(3-1-2-6)	180.0	(8-1-2-4)	180.0			
(8-1-2-6)		0.0							

Frequencies (cm^{-1}): 459.6 584.7 611.3 699.7 740.1 911.9 964.3 1116.5
 1184.7 1223.8 1357.2 1497.0 1512.3 1911.6 3214.6 3215.9 3334.5 3338.4

TS, b3lyp/cc-PVTZ, C_s Geometry

Nuclear repulsion energy	105.526111	Hartree
Zero-point correction	0.057217	Hartree
Thermal correction to Energy	0.061287	Hartree
Thermal correction to Enthalpy	0.062231	Hartree
Thermal correction to Gibbs Free Energy	0.031221	Hartree
B3LYP/cc-PVTZ energy	-191.907567	Hartree
S ²	0.5104	



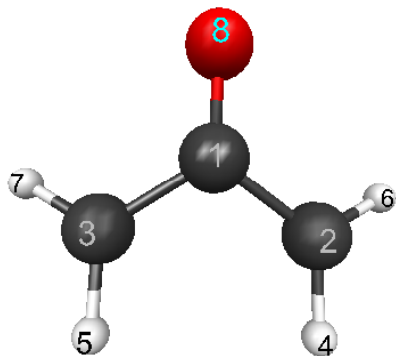
	X	Y	Z
C1	0.076653	-0.175819	0.000000
O2	-0.011157	-1.399936	0.000000
C3	-0.011157	0.684379	1.153929
C4	-0.011157	0.684379	-1.153929
H5	0.447231	1.662611	1.167476
H6	0.447231	1.662611	-1.167476
H7	-0.565616	0.358313	2.024439
H8	-0.565616	0.358313	-2.024439

(1-2)	1.227	(1-3)	1.442	(3-5)	1.080	(3-7)	1.082
(2-1-3)	126.2	(3-1-4)	106.3	(1-3-5)	121.6	(1-3-7)	119.7
(5-3-7)	118.7						
(2-1-3-5)	155.2	(2-1-3-7)	-26.1	(4-1-3-5)	-37.1		
(4-1-3-7)	141.6						

Frequencies (cm⁻¹): -320.1 425.7 490.8 508.0 550.9 784.0 814.5 900.3
942.4 1060.9 1249.3 1460.3 1463.0 1676.3 3139.0 3143.8 3250.5 3255.4

TS, casscf(4/4)/cc-PVTZ, C_s Geometry

Nuclear repulsion energy	105.509366	Hartree
Zero-point correction	0.059887	Hartree
Thermal correction to Enthalpy	0.065855	Hartree
Thermal correction to Gibbs Free Energy	0.031648	Hartree
Casscf(4/4)/cc-PVTZ energy	-190.806201	Hartree
Caspt2(4/4)/cc-PVTZ//casscf(4/4)/cc-PVTZ energy	-191.457438	Hartree



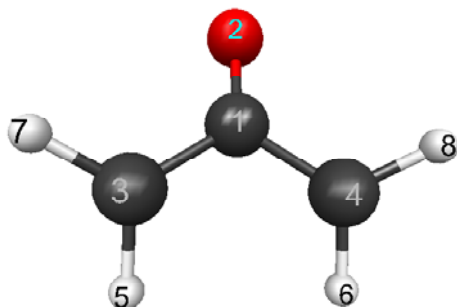
	X	Y	Z
C1	-0.028024	0.157844	0.000000
C2	-0.028024	-0.663731	1.205535
C3	-0.028024	-0.663731	-1.205535
H4	-0.397737	-1.667923	1.188624
H5	-0.397737	-1.667923	-1.188624
H6	0.344532	-0.258196	2.124897
H7	0.344532	-0.258196	-2.124897
O8	0.076355	1.358743	0.000000

(1-2)	1.459	(1-8)	1.205	(2-4)	1.070	(2-6)	1.072
(2-1-3)	111.5	(2-1-8)	124.1	(1-2-4)	121.0	(1-2-6)	119.7
(4-2-6)	119.3						
(3-1-2-4)	-23.8	(3-1-2-6)	156.4	(8-1-2-4)	162.2		
(8-1-2-6)	-17.6						

Frequencies (cm⁻¹): 21.2 409.6 459.9 527.4 543.7 711.0 711.3 926.5
979.5 1144.6 1363.9 1584.7 1585.5 1881.1 3299.8 3305.1 3414.1 3419.5

Radical anion, b3lyp/6-311++G(d,p), C_{2v} Geometry

Nuclear repulsion energy	104.350700 Hartree
Zero-point correction	0.056001 Hartree
Thermal correction to Energy	0.060588 Hartree
Thermal correction to Enthalpy	0.061532 Hartree
Thermal correction to Gibbs Free Energy	0.029733 Hartree
B3LYP/cc-PVTZ energy	-191.972196 Hartree
S ²	0.7716



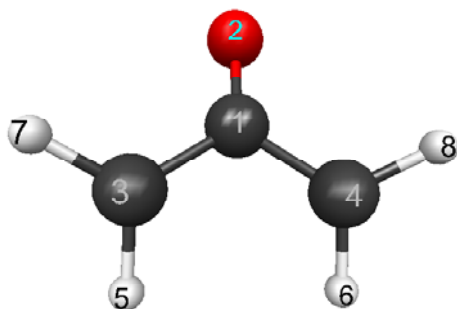
	X	Y	Z
C1	0.000000	0.000000	0.113071
O2	0.000000	0.000000	1.389161
C3	0.000000	1.206052	-0.663632
C4	0.000000	-1.206052	-0.663632
H5	0.000000	1.183566	-1.749185
H6	0.000000	-1.183566	-1.749185
H7	0.000000	2.170470	-0.164881
H8	0.000000	-2.170470	-0.164881

(1-2)	1.276	(1-3)	1.435	(3-5)	1.086	(3-7)	1.086
(2-1-3)	122.8	(3-1-4)	114.4	(1-3-5)	121.6	(1-3-7)	119.9
(5-3-7)	118.5						
(2-1-3-5)	180.0	(2-1-3-7)		0.0	(4-1-3-5)		0.0
(4-1-3-7)	180.0						

Frequencies (cm⁻¹): 384.1 440.1 490.5 492.6 497.9 548.9 700.4 919.3
926.1 1038.6 1162.1 1430.7 1439.0 1511.9 3096.5 3108.2 3193.5 3200.9

Radical anion, b3lyp/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	104.630729 Hartree
Zero-point correction	0.056038 Hartree
Thermal correction to Energy	0.060622 Hartree
Thermal correction to Enthalpy	0.061566 Hartree
Thermal correction to Gibbs Free Energy	0.029778 Hartree
B3LYP/cc-PVTZ energy	-191.972196 Hartree
S ²	0.7716



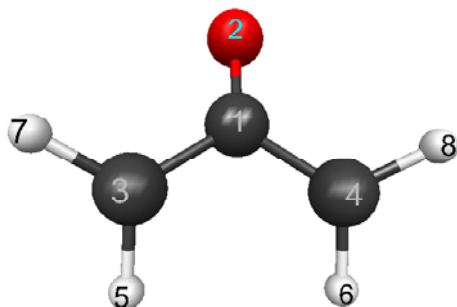
	X	Y	Z
C1	0.000000	0.000000	0.116102
O2	0.000000	0.000000	1.386204
C3	0.000000	1.201083	-0.663400
C4	0.000000	-1.201083	-0.663400
H5	0.000000	1.179574	-1.747066
H6	0.000000	-1.179574	-1.747066
H7	0.000000	2.164338	-0.165655
H8	0.000000	-2.164338	-0.165655

(1-2)	1.270	(1-3)	1.432	(3-5)	1.084	(3-7)	1.084
(2-1-3)	123.0	(3-1-4)	114.0	(1-3-5)	121.8	(1-3-7)	119.7
(5-3-7)	118.5						
(2-1-3-5)	180.0	(2-1-3-7)		0.0	(4-1-3-5)		0.0
(4-1-3-7)	180.0						

Frequencies (cm⁻¹): 393.9 439.1 471.1 483.4 491.7 571.9 718.1 915.2
926.0 1044.6 1154.8 1431.3 1443.1 1549.1 3089.4 3102.1 3182.5 3190.6

Radical anion, b3lyp/aug-cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	104.576982 Hartree
Zero-point correction	0.056328 Hartree
Thermal correction to Energy	0.060835 Hartree
Thermal correction to Enthalpy	0.061779 Hartree
Thermal correction to Gibbs Free Energy	0.030114 Hartree
B3LYP/cc-PVTZ energy	-191.985479 Hartree
S ²	0.7719



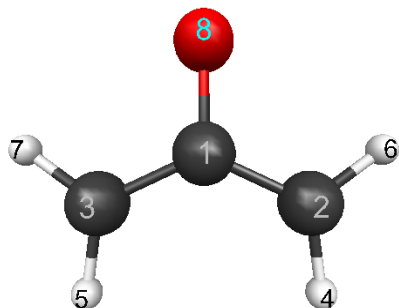
	X	Y	Z
C1	0.000000	0.000000	0.110858
O2	0.000000	0.000000	1.386373
C3	0.000000	1.203582	-0.661591
C4	0.000000	-1.203582	-0.661591
H5	0.000000	1.180597	-1.744328
H6	0.000000	-1.180597	-1.744328
H7	0.000000	2.165799	-0.164192
H8	0.000000	-2.165799	-0.164192

(1-2)	1.276	(1-3)	1.430	(3-5)	1.083	(3-7)	1.083
(2-1-3)	122.7	(3-1-4)	114.6	(1-3-5)	121.5	(1-3-7)	120.0
(5-3-7)	118.6						
(2-1-3-5)	180.0	(2-1-3-7)		0.0	(4-1-3-5)		0.0
(4-1-3-7)	180.0						

Frequencies (cm⁻¹): 400.1 438.7 492.6 508.0 530.0 585.3 716.1 922.4
928.3 1041.4 1167.5 1435.1 1440.9 1506.7 3101.9 3113.2 3194.9 3202.1

Radical anion, casscf(5/4)/cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	105.251327 Hartree
Zero-point correction	0.058022 Hartree
Thermal correction to Enthalpy	0.063575 Hartree
Thermal correction to Gibbs Free Energy	0.032410 Hartree
Casscf(5/4)/cc-PVTZ energy	-190.807871 Hartree
Caspt2(5/4)/cc-PVTZ//casscf(5/4)/cc-PVTZ energy	-191.519894 Hartree



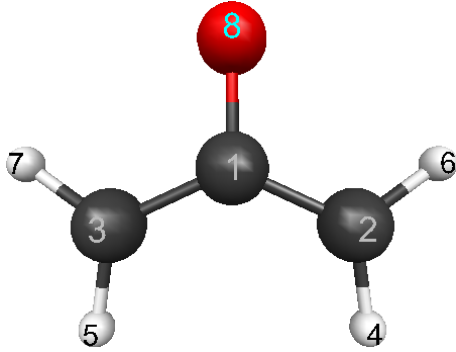
	X	Y	Z
C1	0.000000	0.000000	0.118868
C2	0.000000	1.196382	-0.653356
C3	0.000000	-1.196382	-0.653356
H4	0.000000	1.174430	-1.728393
H5	0.000000	-1.174430	-1.728393
H6	0.000000	2.154285	-0.163876
H7	0.000000	-2.154285	-0.163876
O8	0.000000	0.000000	1.381593

(1-2)	1.424	(1-8)	1.263	(2-4)	1.075	(2-6)	1.076
(2-1-3)	114.3	(2-1-8)	122.8	(1-2-4)	121.7	(1-2-6)	120.1
(4-2-6)	118.2						
(3-1-2-4)	0.0	(3-1-2-6)		180.0	(8-1-2-4)		180.0
(8-1-2-6)	0.0						

Frequencies (cm⁻¹): 396.3 421.8 455.9 469.9 472.2 605.2 723.7 855.4
985.8 1073.6 1119.5 1542.2 1559.5 1639.8 3231.1 3249.5 3320.0 3328.8

Radical anion, casscf(5/4)/aug-cc-PVTZ, C_{2v} Geometry

Nuclear repulsion energy	105.191903 Hartree
Zero-point correction	0.061736 Hartree
Thermal correction to Enthalpy	0.066611 Hartree
Thermal correction to Gibbs Free Energy	0.036439 Hartree
Casscf(5/4)/aug-cc-PVTZ energy	-190.817230 Hartree
Caspt2(5/4)/aug-cc-PVTZ//casscf(5/4)/aug-cc-PVTZ energy	-191.549112 Hartree



	X	Y	Z
C1	0.000000	0.000000	0.113528
C2	0.000000	1.199699	-0.653095
C3	0.000000	-1.199699	-0.653095
H4	0.000000	1.179059	-1.727615
H5	0.000000	-1.179059	-1.727615
H6	0.000000	2.155560	-0.161112
H7	0.000000	-2.155560	-0.161112
O8	0.000000	0.000000	1.379325

(1-2)	1.424	(1-8)	1.266	(2-4)	1.075	(2-6)	1.075
(2-1-3)	114.8	(2-1-8)	122.6	(1-2-4)	121.5	(1-2-6)	120.2
(4-2-6)	118.3						
(3-1-2-4)		0.0	(3-1-2-6)	180.0	(8-1-2-4)		180.0
(8-1-2-6)		0.0					

Frequencies (cm^{-1}): 402.1 426.4 728.2 750.8 789.7 869.6 962.6 1013.9
 1063.8 1087.8 1120.2 1455.9 1479.5 1574.9 3229.4 3243.7 3309.9 3313.6