Appendix D

Geometry Optimizations of the $C_2H_4O_2$ & $C_3H_6O_3$ Structural Isomers

D.1 Introduction

Gaussian 98 MP2 6-311G++(d,p) geometry optimizations were performed for each of the 2C and 3C structural isomers [31]. The rotational constants, dipole moments, and absolute energies determined for the 2C and 3C species are given in Tables D.1 and D.2, respectively, and the resultant relative energy diagrams are shown in Figure D.1. The Gaussian Z-Matrices for each species are presented below.

Table D.1: The 2C structural isomer parameters determined by Gaussian 98 MP2 6-311G++(d,p) geometry optimizations.

Molecule	Energy (hartree)	A (GHz)	B (GHz)	C (GHz)	μ_a	μ_b	μ_c
trans-Acetic Acid	-227.8804311	11.2468400	9.4827443	5.3147628	1.5425	0.0003	-1.2339
cis-Acetic Acid	-227.8697261	10.9315932	9.5932037	5.2786903	2.7307	0.0000	-4.2473
Methyl Formate	-227.8532323	19.8277665	6.9450273	5.3160885	-1.9831	0.0000	-0.1656
Glycolaldehyde	-227.8355319	18.4048626	6.5032670	4.9540965	-1.6280	-0.0572	2.6078

Table D.2: The 3C structural isomer parameters determined by Gaussian 98 MP2 6-311G++(d,p) geometry optimizations.

Molecule	Energy (hartree)	A (GHz)	B (GHz)	C (GHz)	μ_a	μ_b	μ_c
Methylene Glycol Monoformate	-341.8040962	7.60414370	2.3977662	1.9750716	-0.7189	-1.6788	2.1665
Lactic Acid	-341.8035662	5.13517570	3.3496150	2.2075216	-2.4423	0.1351	0.5798
Dimethyl Carbonate	-341.7934922	10.3609486	2.3813303	1.9849098	0.1465	0.0000	0.1066
Methyl Glycolate	-341.7859758	9.95904630	2.2064690	1.8483288	1.3939	2.2628	-1.7720
Methoxy Acetic Acid	-341.7817050	7.56583090	2.3822053	2.0314708	1.9062	1.3609	-0.3790
Glycol Monoformate	-341.7794099	11.2177614	1.8101431	1.6839068	-0.6154	1.6346	0.7070
1,3-Dihydroxyacetone	-341.7676901	9.65454720	2.0397462	1.7323502	0.5000	-1.7533	1.0791
Glyceraldehyde	-341.7634662	5.48513980	2.7894964	2.4086035	1.0842	-2.5990	0.3055
Trioxane	-341.7493150	5.29309690	5.2925296	2.9496941	2.4597	-0.0015	-0.8622

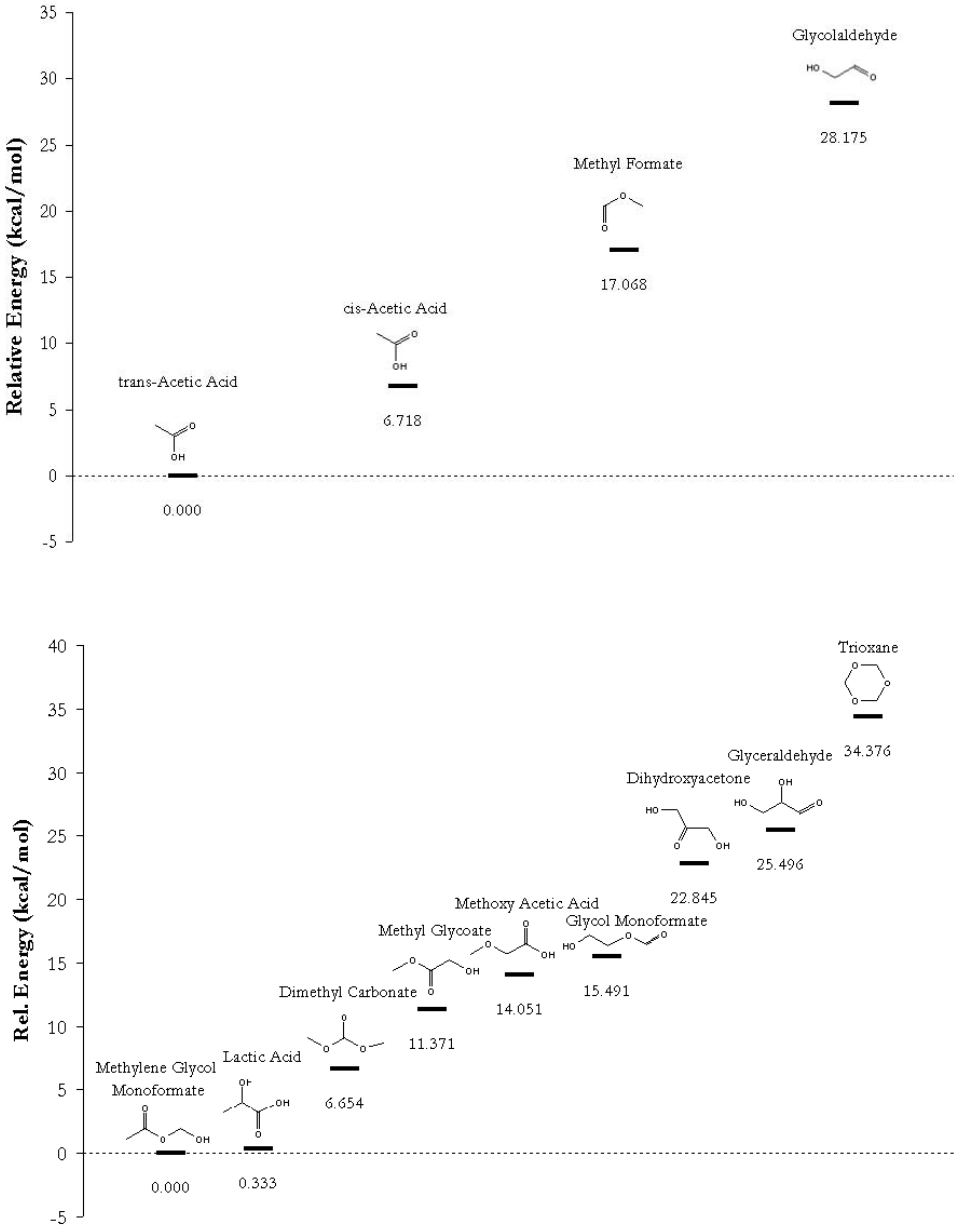

Figure D.1: The relative energies of the $C_2H_4O_2$ (top panel) and $C_3H_6O_3$ (bottom panel) structural isomers.

D.2 Z-Matrices

Table D.3: trans-Acetic Acid Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
C	1	1.503700				
O	2	1.358950	1	111.059625		
H	1	1.088360	2	109.499963	3	179.954742
H	1	1.092271	2	109.523526	3	-59.067658
H	1	1.092264	2	109.529672	3	58.968175
O	2	1.210396	1	126.239110	3	-179.988613
H	3	0.968019	2	105.880805	1	-179.999002

Table D.4: cis-Acetic Acid Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
C	1	1.514811				
O	2	1.365307	1	115.038831		
H	1	1.088383	2	109.211593	3	-179.999852
H	1	1.093990	2	110.171725	3	-59.755578
H	1	1.093990	2	110.171713	3	59.755879
O	2	1.203462	1	124.979429	3	179.999715
H	3	0.963129	2	109.216503	1	-0.000120

Table D.5: Methyl Formate Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
O	1	1.439039				
C	2	1.342820	1	114.123223		
O	3	1.207677	2	125.731253	1	0.000000
H	3	1.097084	2	109.030435	1	-180.000000
H	1	1.087577	2	105.347611	3	-180.000000
H	1	1.091003	2	110.297528	3	60.397010
H	1	1.091003	2	110.297528	3	-60.397010

Table D.6: Glycolaldehyde Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
O						
C	1	1.216358				
C	2	1.509742	1	121.952987		
O	3	1.402974	2	112.266930	1	0.000170
H	4	0.966960	3	105.487287	2	0.011002
H	2	1.105956	1	121.622223	3	-179.995669
H	3	1.099382	2	107.637875	1	122.356765
H	3	1.099397	2	107.631456	1	-122.343986

Table D.7: Methylene Glycol Monoformate Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
C	1	1.525309				
C	2	1.506987	1	111.672591		
O	3	1.215286	2	125.206497	1	8.910305
H	1	1.097583	2	109.626362	3	59.787453
H	1	1.091852	2	109.260546	3	178.184188
O	3	1.351351	2	112.059797	1	-171.585792
H	7	0.968893	3	106.169777	2	-178.343340
H	2	1.095301	1	111.384635	3	-121.586169
H	2	1.095538	1	109.954184	3	119.537879
O	1	1.417311	2	112.140281	3	-64.025342
H	11	0.963865	1	105.429147	2	65.311785

Table D.8: Lactic Acid Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
O						
H	1	0.968758				
C	1	1.348129	2	106.356517		
O	3	1.212801	1	123.875337	2	0.702006
C	3	1.517941	1	112.346787	2	-177.944873
H	5	1.100231	3	106.071131	1	65.847372
C	5	1.523316	3	112.075702	1	-53.644315
H	7	1.091857	5	110.974153	3	63.282595
H	7	1.092065	5	108.681597	3	-176.439566
H	7	1.093130	5	109.916409	3	-57.931883
O	5	1.411925	3	109.827967	1	-175.123445
H	11	0.965841	5	106.474398	3	-15.961845

Table D.9: Dimethyl Carbonate Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
O	1	1.338797				
O	1	1.338797	2	107.820415		
C	2	1.435114	1	113.502682	3	179.999999
H	4	1.091117	2	110.509182	1	60.607259
H	4	1.091117	2	110.509182	1	-60.607259
H	4	1.087999	2	105.142494	1	180.000000
C	3	1.435114	1	113.502682	2	-180.000000
H	8	1.091117	3	110.509182	1	-60.607259
H	8	1.091117	3	110.509182	1	60.607259
H	8	1.087999	3	105.142495	1	180.000000
O	1	1.210758	2	126.089792	4	0.000000

Table D.10: Methyl Glycolate Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
C	1	1.515309				
H	2	1.095651	1	108.205654		
H	2	1.095618	1	108.217122	3	116.773821
O	1	1.338913	2	111.747328	4	58.316900
O	1	1.214318	2	123.352467	5	-179.992768
O	2	1.407602	1	111.096393	6	-0.067947
H	7	0.965986	2	105.821878	1	0.134171
C	5	1.439953	1	114.560283	2	179.987660
H	9	1.087693	5	105.250932	1	-179.999743
H	9	1.090889	5	110.213053	1	-60.468310
H	9	1.090887	5	110.213301	1	60.468843

Table D.11: Methoxy Acetic Acid Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
O	1	1.420513				
C	2	1.396539	1	112.311695		
C	3	1.522851	2	113.504856	1	-74.996247
O	4	1.206939	3	126.557079	2	-0.069676
O	4	1.357945	3	109.623802	2	-179.576155
H	6	0.968236	4	106.261800	3	178.980760
H	3	1.093625	2	107.673258	1	166.083302
H	3	1.100786	2	112.134344	1	47.772178
H	1	1.098690	2	110.522883	3	-58.480384
H	1	1.094190	2	111.496974	3	63.843977
H	1	1.089885	2	106.539316	3	-177.024465

Table D.12: Glycol Monoformate Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
C	1	1.528415				
O	2	1.412307	1	114.347702		
O	1	1.453147	2	114.056725	3	97.769306
C	4	1.333737	1	116.631752	2	-68.334659
O	5	1.212591	4	126.243317	1	3.172829
H	5	1.096436	4	109.414019	1	-176.883010
H	1	1.093622	2	110.171399	3	-25.408419
H	1	1.090205	2	110.732082	3	-147.052458
H	2	1.099672	1	108.445413	4	-28.041192
H	2	1.093073	1	108.114766	4	-144.662847
H	3	0.965246	2	106.211583	1	-51.688895

Table D.13: 1,3-Dihydroxyacetone Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
C	1	1.514665				
H	2	1.101962	1	106.409456		
H	2	1.095236	1	109.780776	3	-116.049712
C	1	1.514675	2	118.405260	4	-42.162081
H	5	1.095158	1	109.801311	2	-42.045849
H	5	1.101966	1	106.406408	2	74.025658
O	1	1.221370	2	120.796268	5	179.983688
O	5	1.404249	1	112.130211	2	-163.446551
H	9	0.966185	5	105.762029	1	-25.060504
O	2	1.404121	1	112.136696	8	16.399881
H	11	0.966200	2	105.767937	1	-24.788882

Table D.14: Glyceraldehyde Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
C	1	1.523478				
H	2	1.096842	1	108.597282		
H	2	1.093765	1	110.256321	3	-118.906916
C	1	1.516183	2	110.674020	4	59.015863
H	5	1.105654	1	116.435269	2	-53.308715
O	1	1.410485	2	108.592495	5	121.450366
H	7	0.968698	1	105.546873	2	-134.748948
O	5	1.215756	1	121.710439	2	127.677466
O	2	1.415281	1	110.684405	7	62.245137
H	10	0.964149	2	105.704544	1	-56.062409
H	1	1.103124	2	109.028659	10	-176.653874

Table D.15: Trioxane Z-Matrix.

Atom 1	Atom 2	Bond (Å)	Atom 3	Angle (°)	Atom 4	Dihedral Angle (°)
C						
H	1	1.087341				
H	1	1.103708	2	111.408314		
O	1	1.408253	2	107.615748	3	-119.919101
O	1	1.408837	2	107.584294	4	-120.237198
C	4	1.408777	1	108.644724	2	-176.275190
H	6	1.087343	4	107.585058	1	176.325387
H	6	1.103731	4	109.354212	1	-62.538123
C	5	1.407974	1	108.649293	2	176.311887
H	9	1.103746	5	109.418694	1	62.517471
H	9	1.087351	5	107.624267	1	-176.292182
O	6	1.408328	4	111.471551	1	58.553254