Supporting Information for

Identification of Glycolaldehyde Enol (HOHC=CHOH) in Interstellar Analog Ices

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Error determination of computed ionization energies

As the identification of different isomers in our studies focusses on the ionization energy of each isomer, we performed additional ionization energy computations at the same level of theory for multiple oxygen-containing complex organic molecules as benchmarks (Table S8). Error bounds were determined by subtracting the calculated ionization energy from the error boundaries of the experimentally determined and hence known values for each molecule. Afterwards, the average difference to the lower and upper boundary as well as their standard deviation were calculated. Finally, the standard deviation was subtracted from or added to the average difference for the lower and upper boundary, respectively. This conservative analysis yielded errors of −0.06/+0.11 eV, which allows us to distinguish all isomers of interest in this study based on their calculated and/or experimentally determined ionization energy.

CO-CH_3OH ratio determination

To quantify the ratio of the ice constituents, methanol and carbon monoxide ices of known thicknesses were prepared and IR spectra were taken to determine the absorption coefficient. This absorption coefficient was then used along with a modified Lambert-Beer law to determine the column densities of the ice constituents. The CO stretching and CH_3 rocking mode (1040 cm^{-1}; 1027 cm^{-1}, combined absorption coefficient A = 1.6 × 10^{-18} cm $molecule^{-1}$), the CH_3 rocking mode at 1129 cm^{-1} (A = 2.1 × 10^{-19} cm $molecule^{-1}$), and the CH deformation and OH bending mode at 1460 cm^{-1} (A = 1.1 × 10^{-18} cm $molecule^{-1}$) of methanol were used for the determination of the column density of methanol along with the CO stretching mode of carbon monoxide at 2136 cm^{-1} (A = 1.2 × 10^{-18} cm $molecule^{-1}$) to determine its column density. For all binary ices in this study, this analysis yielded a carbon monoxide to methanol ratio of 1:1.2 ± 0.2. The uncertainty was determined by the standard deviation of the column densities determined by individual IR modes and the standard deviation of the ratio across all ices prepared.

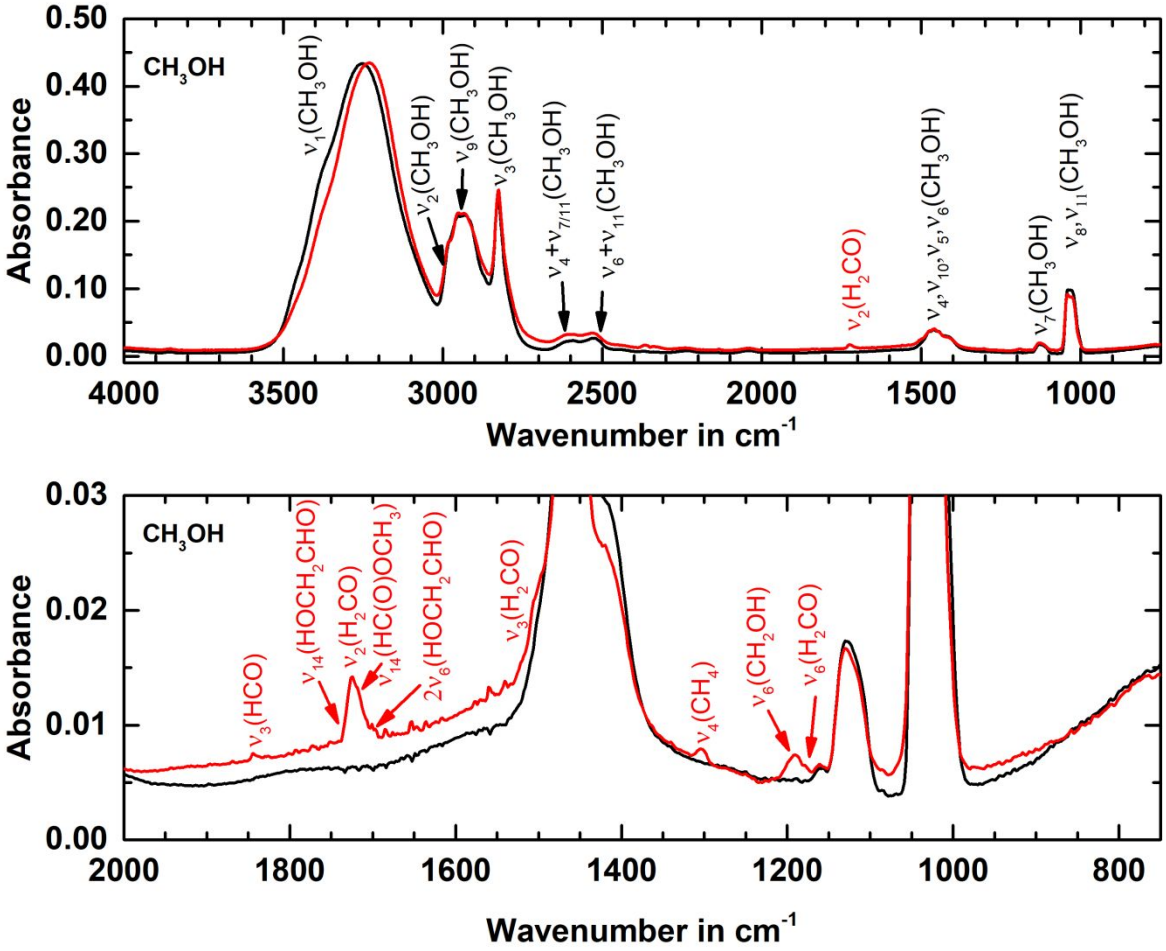


Figure S1: IR spectra of pure methanol ice before (black lines) and after irradiation (red lines). Spectra are slightly offset to highlight differences. Red labels indicate newly formed molecules.

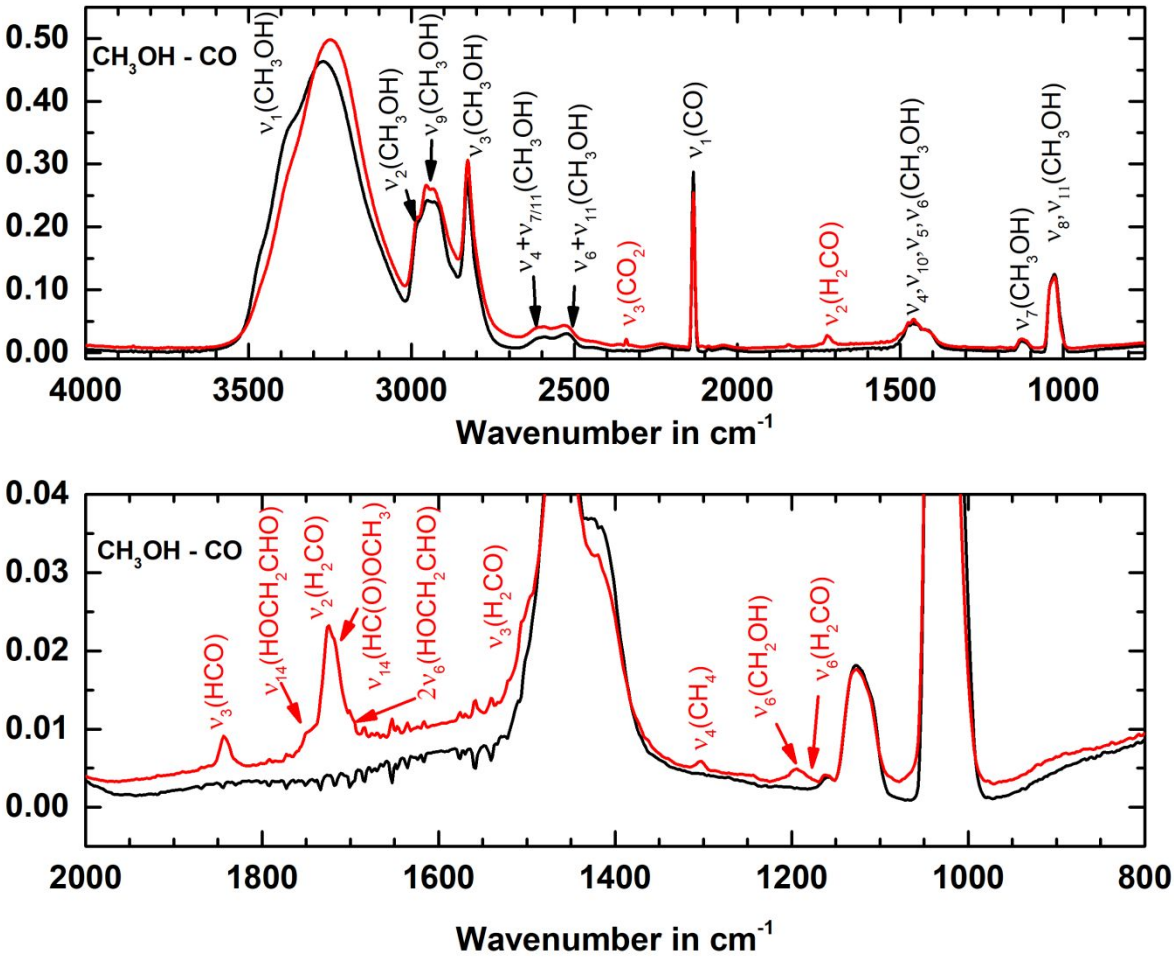


Figure S2: IR spectra of methanol-carbon monoxide ice before (black lines) and after irradiation (red lines). Spectra are slightly offset to highlight differences. Red labels indicate newly formed molecules.

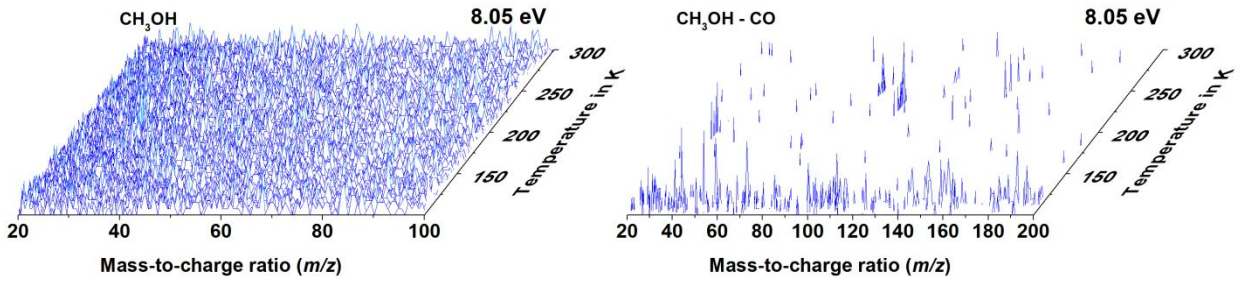


Figure S3: Temperature-dependent time-of-flight mass spectra of pure methanol ice (left) and methanol – carbon monoxide ice (right) after electron irradiation recorded at 8.05 eV.

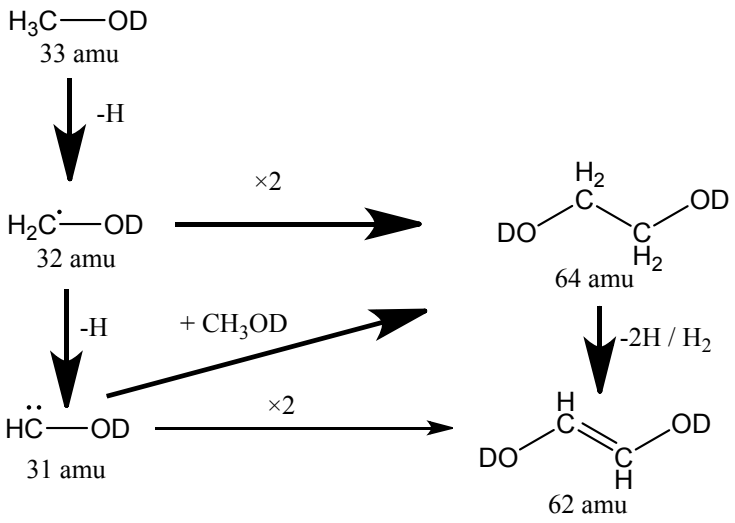


Figure S4: Reaction pathways inferred from isotopically labelled methanol-OD. Thick arrows designate the pathways considered relevant for the formation of 1,2-ethenediol.

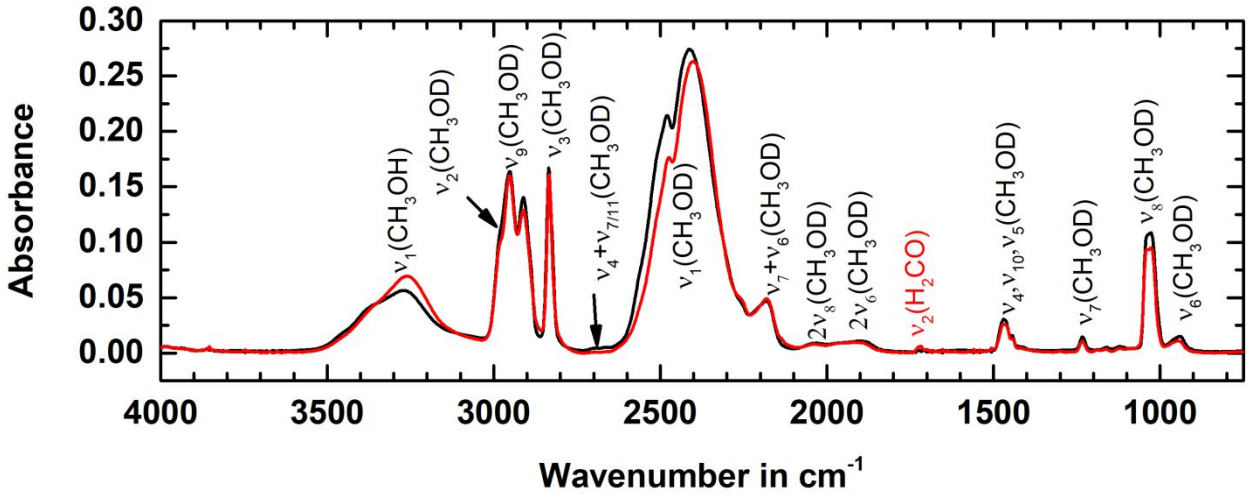


Figure S5: IR spectra of methanol-OD before (black lines) and after irradiation (red lines). Red labels indicate newly formed molecules. Modes are numbered according to their order in regular methanol.

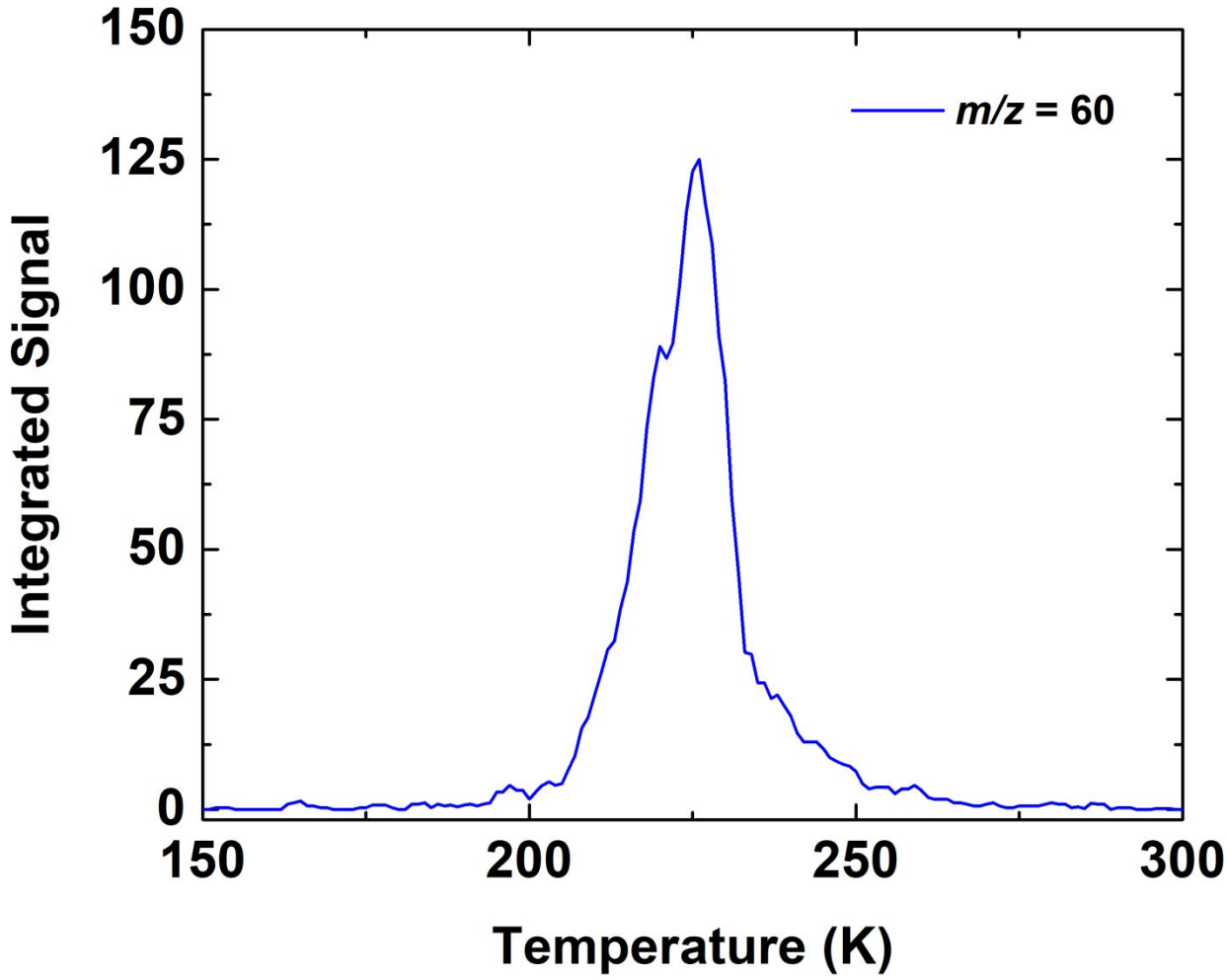


Figure S6: Desorption profile of *m/z* -= 60 ($C_2H_4O_2$) in irradiated ethylene glycol ($(CH_2OH)_2$) recorded at a photon energy of 8.50 eV. The resulting ion signal can only be due to 1,2-ethenediol.

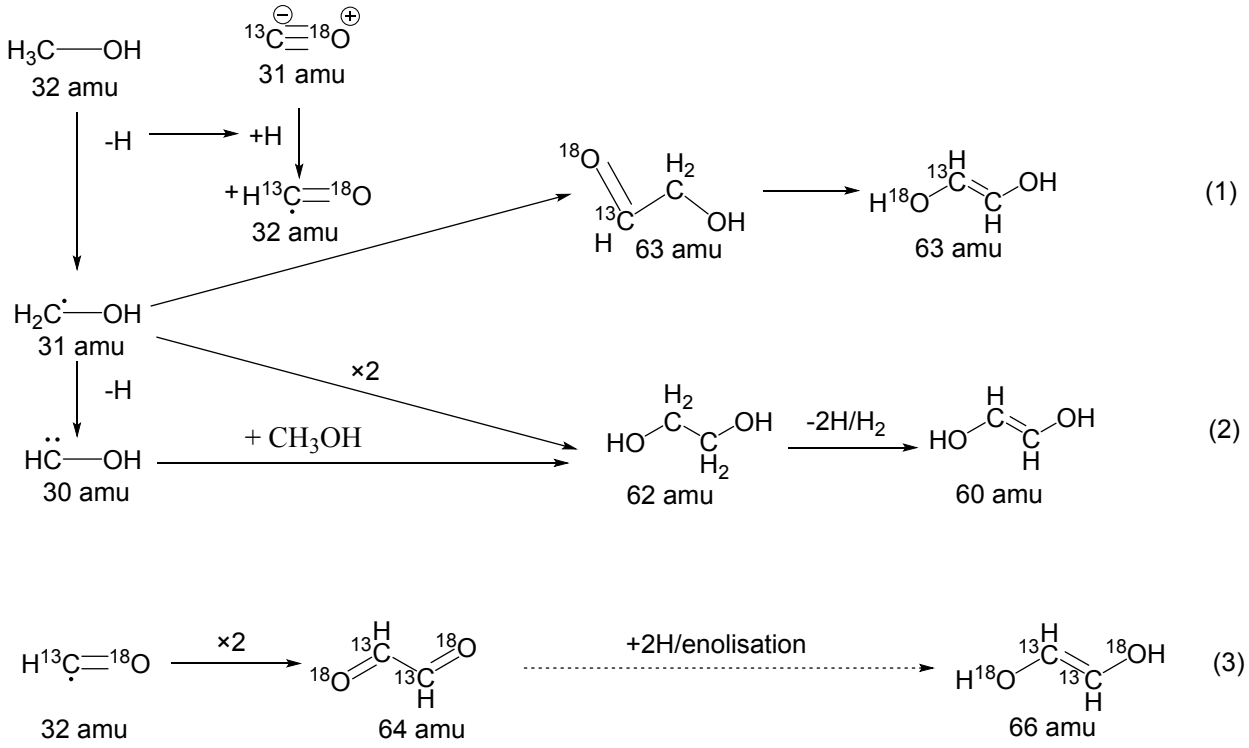


Figure S7. Reaction pathways inferred from isotopically labelled methanol-$^{13}C^{18}O$. The dashed arrows define the overall process excluding reactive radical intermediates.

Table S1: Computed relative energies and dipole moments for 1,2-ethenediol conformers at B3LYP/cc-pVTZ level of theory.

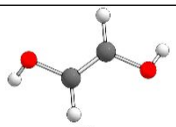
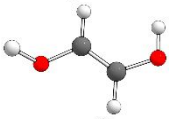
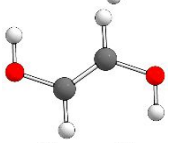
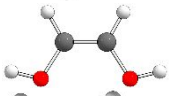
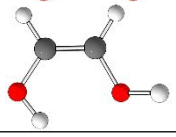
Structure	Name	Point group	Electronic state	Rel. energy in kJ mol^{-1}	Dipole moment μ in Debye
	*E-anti-anti*-1,2-ethenediol	C_2	^{1}A	18	1.28
	*E-syn-anti*-1,2-ethenediol	C_1	^{1}A	17	2.36
	*E-syn-syn*-1,2-ethenediol	C_2	^{1}A	15	0.00
	*Z-anti-anti*-1,2-ethenediol	C_{2v}	^{1}A$_1$	15	2.13
	*Z-syn-anti*-1,2-ethenediol	C_1	^{1}A$_1$	0	2.25

Table S2: Data used to calculate irradiation doses.

Parameter	CH_3OH	CH_3OH - CO	
irradiation current, I (nA)	30 ± 2	30 ± 2	
initial kinetic energy of the electrons, E_{init}	5 keV	5 keV	
total number of electrons	$(6.7 \pm 0.3)\times10^{14}$	$(6.7 \pm 0.3)\times10^{14}$	
average penetration depth, l^* (nm)	260 ± 30	280 ± 30	
density of the ice, ρ (g cm^{-3})	1.020	1.023	
average kinetic energy of transmitted electrons, E_{trans}^* (keV)	0	0	
average kinetic energy of backscattered electrons, E_{bs}^* (keV)	3.2 ± 0.3	3.3 ± 0.3	
fraction of transmitted electrons, f_{trans}^*	0	0	
fraction of backscattered electrons, f_{bs}^*	0.33 ± 0.03	0.35 ± 0.03	
irradiated area, A (cm^2)	1.0 ± 0.1	1.0 ± 0.1	
molecule	CH_3OH	CH_3OH	CO
total # molecules processed	$(5.0\pm 0.7)\times10^{17}$	$(3.1 \pm 0.5)\times10^{17}$	$(2.5 \pm 0.3)\times10^{17}$
dose per molecule (eV)	5.3 ± 0.8	4.9 ± 0.8	4.2 ± 0.7

Notes: *CASINO output values

Table S3: Wavelengths and dyes used to generate the different photon energies of the photoionization source.

	Photon energy (eV)	9.75	8.82	8.50	8.05
	Wavelength (nm)	127.2	140.6	145.9	154.0
ω_1	Wavelength (nm)	202.316	222.566	202.316	249.628
Nd:YAG (ω_1)	Wavelength (nm)	532	355	532	355
Dye laser (ω_1)	Wavelength (nm)	606.948	445.132	606.948	499.256
Dye (ω_1)[a]		Rh mix	C 450	Rh mix	C 503
ω_2	Wavelength (nm)	495	534	330	658
Nd:YAG (ω_2)	Wavelength (nm)	355	355	532	532
Dye laser (ω_2)	Wavelength (nm)	495	534	660	658
Dye (ω_2)[a]		C 503	C 540 A	DCM	DCM

Notes: [a] Rh mix: Rhodamine 610 + Rhodamine 640, C 450/503/540 A: Coumarin 450/503/540 A

Table S4: Infrared absorptions in methanol and methanol-OD ices before and after irradiation.

CH_3OH		CH_3OD		Assignment	Mode
Before irradiation cm^{-1}	After irradiation cm^{-1}	Before irradiation cm^{-1}	After irradiation cm^{-1}		
4398		4407		$\nu_2/\nu_9+\nu_4/\nu_6/\nu_{10}(CH_3OH)$	Combination
4275		4276		$\nu_2/\nu_9+\nu_4(CH_3OH)$	Combination
4020		4015		$\nu_2/\nu_9+\nu_8(CH_3OH)$	Combination
3989		3984		$\nu_2/\nu_9+\nu_8(CH_3OH)$	Combination
3600-3020		2600-2100		$\nu_1(CH_3OH)$	OH Stretching
			2253	unknown	
2985		2985		$\nu_2(CH_3OH)$	CH_3 asym. str.
2950		2950		$\nu_9(CH_3OH)$	CH_3 symm. str.
2925				$\nu_4+\nu_5/\nu_4+\nu_{10}/\nu_5+\nu_{10}/2\nu_4/2\nu_{10}/2\nu_5$ (CH_3OH)	Combination/ Overtone
2825		2825		$\nu_3(CH_3OH)$	CH_3 sym. Str.
2604		2605		$\nu_4+\nu_{11}/\nu_7+\nu_4/\nu_6/\nu_{10}$ (CH_3OH)	Combination
2526				$\nu_6+\nu_{11}(CH_3OH)$	Combination
	2340			$\nu_3(CO_2)$	C=O stretch
2235				$2\nu_{11}/2\nu_7$ (CH_3OH)	Overtone
		2185		$\nu_7+\nu_6$ (CH_3OD)	Overtone
	2134			$\nu_1(CO)$	CO stretch
2040		2040		$2\nu_8(CH_3OH)$	Overtone
		1895		$2\nu_6(CH_3OD)$	Overtone
	1844			$\nu_3(HCO)$	C=O stretch
	1750			$\nu_{14}(HOCH_2CHO)$	
	1726		1721	$\nu_2(H_2CO)$	C=O stretch
	1718		1716	$\nu_{14}(HC(O)OCH_3)$	C=O stretch
	1700			$2\nu_6(HOCH_2CHO)$	
	1508			$\nu_3(H_2CO)$	CH_2 scissor
	1499			$\nu_3(H_2CO)$	CH_2 scissor
1477		1469		$\nu_4(CH_3OH)$	CH_3 asym. bend
1461		1461		$\nu_{10}(CH_3OH)$	CH_3 asym. bend
1445		1445		$\nu_5(CH_3OH)$	CH_3 symm bend
1420		940		$\nu_6(CH_3OH)$	O-H bend
	1302		1301	$\nu_4(CH_4)$	deformation
		1233			CH_3 rocking
	1192		1190	$\nu_6(CH_2OH)$	CO stretch
	1177			$\nu_6(H_2CO)$	CH_2 wagging
1135		1160		$\nu_7(CH_3OH)$	CH_3 rocking
1123		1120		$\nu_7(CH_3OH)$	CH_3 rocking
	1092		1092	$\nu_2(HCO)$	bending
1040		1040		$\nu_{11}(CH_3OH)$	CH_3 rocking

1026	1027	$\nu_8(CH_3OH)$	CO stretch
667		$\nu_2(CO_2)$	C=O bend

Table S5: Infrared absorptions in methanol – carbon monoxide and methanol – carbon monoxide-$^{13}C^{18}O$ ices before and after irradiation.

CH_3OH-CO		CH_3OH-$^{13}C^{18}O$		Assignment	Mode
Before irradiation cm^{-1}	After irradiation cm^{-1}	Before irradiation cm^{-1}	After irradiation cm^{-1}		
4400		4402		$\nu_2/\nu_9+\nu_4/\nu_6/\nu_{10}(CH_3OH)$	Combination
4277		4278		$\nu_2/\nu_9+\nu_4(CH_3OH)$	Combination
		4049			
4017		4016		$\nu_2/\nu_9+\nu_8(CH_3OH)$	Combination
3986		3984		$\nu_2/\nu_9+\nu_8(CH_3OH)$	Combination
3600-3020		3600-3200		$\nu_1(CH_3OH)$	OH Stretching
2985		2985		$\nu_2(CH_3OH)$	CH_3 asym. str.
2953		2954		$\nu_9(CH_3OH)$	CH_3 sym. str.
2925		2922		$\nu_4+\nu_5/\nu_4+\nu_{10}/\nu_5+\nu_{10}/2\nu_4/2\nu_{10}/2\nu_5$ (CH_3OH)	Combination/ Overtone
2827		2829		$\nu_3(CH_3OH)$	CH_3 sym. Str.
		2615		$\nu_4+\nu_{11}/\nu_7+\nu_4/\nu_6/\nu_{10}$ (CH_3OH)	Combination
2604		2591		$\nu_4+\nu_{11}/\nu_7+\nu_4/\nu_6/\nu_{10}$ (CH_3OH)	Combination
2523		2522		$\nu_6+\nu_{11}(CH_3OH)$	Combination
			2361	$\nu_3(CO_2)$	C=O stretch
	2340		2340	$\nu_3(CO_2)$	C=O stretch
			2275	$\nu_3(^{13}CO_2)$	C=O stretch
			2258	$\nu_3(^{13}C^{16}O^{18}O)$	C=O stretch
			2239	$\nu_3(^{13}C^{18}O_2)$	C=O stretch
2235				$2\nu_{11}/2\nu_7$ (CH_3OH)	Overtone
2136			2136	$\nu_1(CO)$	CO stretch
	2107			unknown	
2088		2088		$\nu_1(^{13}CO/C^{18}O)$	CO stretch
		2038		$\nu_1(^{13}C^{18}O)$	CO stretch
2044				$2\nu_8(CH_3OH)$	Overtone
	1843			$\nu_3(HCO)$	C=O stretch
	1750			$\nu_{14}(HOCH_2CHO)$	
	1726		1721	$\nu_2(H_2CO)$	C=O stretch
	1718		1712	$\nu_{14}(HC(O)OCH_3)$	C=O stretch
	1700			$2\nu_6(HOCH_2CHO)$	
	1504		1507	$\nu_3(H_2CO)$	CH_2 scissor
	1499		1499	$\nu_3(H_2CO)$	CH_2 scissor
1475		1475		$\nu_4(CH_3OH)$	CH_3 asym. bend
1461		1461		ν_{10} (CH_3OH)	CH_3 asym. bend
1445		1445		$\nu_5(CH_3OH)$	CH_3 sym. bend
1421		1421		$\nu_6(CH_3OH)$	O-H bend
	1302		1304	ν_3 (CH_4)	Deg. str.
	1211				COH deform.

	1193		1192	ν_6 (CH_2OH)	CO stretch
	1177		1177	ν_6 (H_2CO)	CH_2 wagging
1158		1161		ν_7(CH_3OH)	CH_3 rocking
1126		1125		ν_7(CH_3OH)	CH_3 rocking
1110		1110		ν_7(CH_3OH)	CH_3 rocking
	1092			ν_2(HCO)	bending
1040		1040		ν_{11}(CH_3OH)	CH_3 rocking
1027		1027		ν_8 (CH_3OH)	CO stretch
	667		667	ν_2(CO_2)	C=O bend

Table S6. Infrared frequencies and intensities of 1,2-ethenediol conformers at CCSD(T)/cc-pWCVTZ level of theory

E-anti-anti		*E-syn-anti*		*E-syn-syn*	
Frequency in cm^{-1}	Intensity	Frequency in cm^{-1}	Intensity	Frequency in cm^{-1}	Intensity
155.9	98.4	230.8	128.1	226.2	122.1
243.3	150.6	285.4	25.8	277.4	0.0
326.1	15.3	321.2	17.9	315.1	34.1
328.5	29.4	391.8	69.7	367.0	68.0
574.0	2.2	570.1	8.0	566.7	0.0
801.5	3.3	787.1	11.5	784.2	0.0
913.9	56.6	932.1	62.2	907.5	83.8
1109.7	0.2	1102.4	92.4	1082.9	0.0
1166.9	382.1	1171.3	262.5	1152.1	368.7
1216.3	71.3	1225.2	30.6	1233.4	7.8
1278.8	1.1	1316.9	3.5	1333.2	0.0
1345.8	0.0	1335.2	18.0	1366.7	0.0
1400.8	13.3	1407.7	39.7	1424.5	99.9
1779.7	0.3	1753.7	11.2	1747.7	0.0
3183.2	26.4	3142.3	30.1	3203.5	27.3
3187.6	0.0	3233.6	5.3	3204.0	0.0
3868.4	122.3	3830.4	34.4	3835.4	70.3
3870.0	16.3				

Z-anti-anti		*Z-syn-anti*	
Frequency in cm^{-1}	Intensity	Frequency in cm^{-1}	Intensity
80.9	0.0	221.1	78.4
93.7	196.0	257.9	60.0
240.0	3.7	471.9	55.8
524.4	0.0	549.0	74.5
713.1	78.8	725.6	37.7
728.9	33.8	766.5	28.1
826.2	0.0	874.4	9.1
1024.5	10.1	1032.9	39.9
1131.1	135.4	1122.5	146.8
1230.8	127.7	1214.2	30.7
1315.9	86.2	1275.0	110.3
1326.7	92.8	1380.8	2.7
1454.0	28.2	1439.6	55.2
1799.6	20.5	1753.3	51.2
3201.5	0.9	3218.1	4.5
3225.4	18.9	3253.8	9.9
3889.6	156.6	3789.0	49.9

Table S7: Computed adiabatic ionization energies and relative energies for $C_2H_4O_2$ isomers at CCSD(T)/CBS//B3LYP/cc-pVTZ level of theory + zero-point vibrational energy.

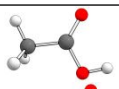
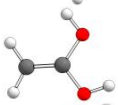
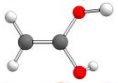
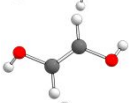
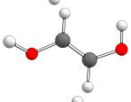
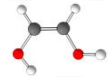
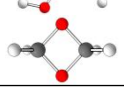
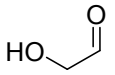
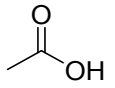
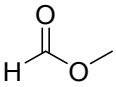
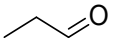
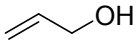
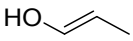
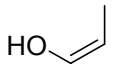
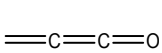
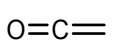
Structure	Name	IE_{calc} in eV	IE_{exp} in eV	Electronic state	Relative energy in kJ mol^{-1}
	*anti*-acetic acid	10.65	10.65 ± 0.02[1]	^{1}A'	0
	*syn*-acetic acid	10.52		^{1}A'	21
	*syn, syn*-1,1-ethenediol	8.68		^{1}A$_1$	117
	*syn, anti*-1,1-ethenediol	8.58		^{1}A'	112
	*anti, anti*-1,1-ethenediol	8.59		^{1}A	125
	*anti*-methyl formate	10.68	10.835[1]	^{1}A'	93
	*syn*-methyl formate	10.83		^{1}A'	73
	*syn*, *syn*-glycolaldehyde	10.06		^{1}A'	113
	*syn*, *anti*-glycolaldehyde	9.84	9.95 ±0.05[2]	^{1}A'	134
	*anti*, *anti*-glycolaldehyde	9.91		^{1}A'	126
	*anti*, *gauche*-glycolaldehyde	9.90		^{1}A	127
	*E-anti-anti*-1,2-ethenediol	8.16		^{1}A	167
	*E-syn-anti*-1,2-ethenediol	8.30		^{1}A	166
	*E-syn-syn*-1,2-ethenediol	8.41		^{1}A	165
	*Z-anti-anti*-1,2-ethenediol	8.21		^{1}A$_1$	162
	*Z-syn-anti*-1,2-ethenediol	8.37		^{1}A	147
	*Oxiran-2-ol*	8.93		^{1}A	195
	*1,3-Dioxetane*	10.08		^{2}B$_{1u}$	235

Table S8: Error analysis of computed ionization energies for COMs containing one and two oxygen atoms; adiabatic ionization energies were computed at CCSD(T)/CBS//B3LYP/cc-pVTZ level of theory + zero-point vibrational energy.

Structure	Name	Experimental adiabatic ionization energy in eV	Lowest Computed adiabatic ionization energy in eV	Difference to lower bound	Difference to upper bound
	Glycolaldehyde	9.95 ±0.05 [2]	9.84	0.06	0.16
	Acetic Acid	10.65 ± 0.02 [1]	10.52	0.11	0.15
	Methyl Formate	10.835 [1]	10.68	0.155	0.155
	Acetone	9.703 ± 0.006 [1]	9.71	−0.013	−0.001
	Propanal	9.96 ± 0.01 [1]	9.97	-0.02	0.00
	Propylene oxide	10.22 ± 0.02 [3]	10.24	−0.04	0.00
	Prop-1-en-2-ol	8.67 ± 0.05 [4]	8.71	−0.09	0.01
	2-Propen-1-ol	9.67 ± 0.03 [1]	9.65	−0.01	0.05
	(*E*)-1-Propenol	8.64 ± 0.02 [5]	8.61	0.01	0.05
	(*Z*)-1-Propenol	8.70 ± 0.03 [5]	8.63	0.04	0.10
	Methanol	10.84 ± 0.01	10.86	−0.03	−0.01
	Propadienone	9.12 ± 0.05	9.15	−0.08	0.02
	Formaldehyde	10.88 ± 0.01	10.89	−0.02	0.00
	Ketene	9.617 ± 0.003	9.58	0.034	0.040
	Acetaldehyde	10.229 ± 0.0007	10.24	−0.0117	−0.0103
			Average difference	0.006	0.048
			Std. deviation	0.066	0.063
			Error bounds	−0.06	0.11

Cartesian Coordinates for Selected Structures of $C_2H_4O_2$

B3LYP/cc-pVTZ optimized geometry (distances in Å), electronic energies (in hartree), zero-point vibrational energies (ZPVE), extrapolated CCSD(T)/CBS energies (in hartree) and adiabatic ionization energies (IE) at CCSD(T)/CBS//B3LYP/cc-pVTZ level of theory.

cis Acetic acid cation (C_s)

C	–1.012317	–0.964938	0.000000
C	0.064451	0.082674	0.000000
H	–2.006868	–0.521206	0.000000
H	–0.879238	–1.565654	0.905304
H	–0.879238	–1.565654	–0.905304
O	–0.373776	1.254641	0.000000
O	1.327467	–0.121447	0.000000
H	1.576888	–1.063412	0.000000

E = –228.7951578
E[CCSD(T)/CBS] = –228.4591383
ZPVE = 157.0305 kJ mol^{-1}

cis Acetic acid (C_s)

C	1.384403	–0.444093	0.000000
C	–0.020669	0.115577	0.000000
H	2.097845	0.373595	0.000000
H	1.547860	–1.065592	–0.882491
H	1.547860	–1.065592	0.882491
O	–0.293502	1.280081	0.000000
O	–1.016092	–0.815392	0.000000
H	–0.647118	–1.705775	0.000000

E = –229.1725686
E[CCSD(T)/CBS] = –228.8472353
ZPVE = 161.1038 kJ mol^{-1}

trans Acetic acid cation (C_s)

C	–1.081166	–0.903862	0.000000
C	0.045594	0.071434	0.000000
H	–2.051782	–0.410721	0.000000
H	–0.965779	–1.515243	0.901193
H	–0.965779	–1.515243	–0.901193

O	–0.266434	1.282335	0.000000
O	1.263657	–0.338800	0.000000
H	1.939045	0.369124	0.000000

E = –228.7985722
E[CCSD(T)/CBS] = –228.4616873
ZPVE = 156.0637 kJ mol^{-1}

trans Acetic acid (C_s)

C	1.423315	–0.312362	0.000000
C	–0.019649	0.106963	0.000000
H	2.057643	0.567904	0.000000
H	1.631074	–0.924037	–0.877888
H	1.631074	–0.924037	0.877888
O	–0.427736	1.238677	0.000000
O	–0.850028	–0.965037	0.000000
H	–1.753960	–0.617026	0.000000

E = –229.1811770
E[CCSD(T)/CBS] = –228.8554091
ZPVE = 161.7909 kJ mol^{-1}

cis, *cis* 1,1-Ethenediol cation (C_{2v})

C	0.000000	0.000000	0.025454
C	0.000000	0.000000	1.443455
H	0.000000	–0.942538	1.969724
H	0.000000	0.942538	1.969724
O	0.000000	1.146808	–0.577470
H	0.000000	1.133094	–1.549871
O	0.000000	–1.146808	–0.577470
H	0.000000	–1.133094	–1.549871

E = –228.8255200
E[CCSD(T)/CBS] = –228.4916277
ZPVE = 159.9339 kJ mol–1

cis, *cis* 1,1-Ethenediol (C_2)

C	0.000000	0.000000	–0.079487
C	0.000000	0.000000	–1.404595
H	–0.931416	0.055195	–1.942827
H	0.931416	–0.055195	–1.942827

O	1.128211	–0.212864	0.661238
H	1.132941	0.402815	1.404760
O	–1.128211	0.212864	0.661238
H	–1.132941	–0.402815	1.404760

E = –229.1326146
E[CCSD(T)/CBS] = –228.8072804
ZPVE = 160.0441 kJ mol^{-1}

cis, *trans* 1,1-Ethenediol cation (C_s)

C	–0.014571	0.005326	0.000000
C	–0.391208	1.375179	0.000000
H	0.382768	2.128613	0.000000
H	–1.432608	1.663026	0.000000
O	–0.840287	–0.993688	0.000000
H	–1.780303	–0.747631	0.000000
O	1.242361	–0.276385	0.000000
H	1.426254	–1.235319	0.000000

E = –228.8304016
E[CCSD(T)/CBS] = –228.4968440
ZPVE = 160.6893 kJ mol^{-1}

cis, *trans* 1,1-Ethenediol (C_s)

C	0.000000	0.023323	–0.077490
C	0.000000	–0.005160	–1.408088
H	0.000000	0.915395	–1.966530
H	0.000000	–0.942638	–1.940970
O	0.000000	–1.057705	0.752872
H	0.000000	–1.863932	0.227096
O	0.000000	1.165684	0.639497
H	0.000000	0.933426	1.575090

E = –229.1373598
E[CCSD(T)/CBS] = –228.8118010
ZPVE = 159.5802 kJ mol^{-1}

trans, trans 1,1-Ethenediol cation (C_{2v})

C	0.000000	0.000000	–0.019064
C	0.000000	0.000000	1.406857
H	0.000000	0.930956	1.956399

H	0.000000	–0.930956	1.956399
O	0.000000	–1.071954	–0.736537
H	0.000000	–1.898631	–0.227486
O	0.000000	1.071954	–0.736537
H	0.000000	1.898631	–0.227486

E = –228.8243955
E[CCSD(T)/CBS] = –228.4913406
ZPVE = 160.4209 kJ mol^{-1}

trans, trans 1,1-Ethenediol (C_{2v})

C	0.000000	0.000000	–0.071731
C	0.000000	0.000000	–1.408140
H	0.000000	0.924602	–1.963761
H	0.000000	–0.924602	–1.963761
O	0.000000	–1.089183	0.725564
H	0.000000	–1.876169	0.172050
O	0.000000	1.089183	0.725564
H	0.000000	1.876169	0.172050

E = –229.1356581
E[CCSD(T)/CBS] = –228.8102922
ZPVE = 160.4708 kJ mol^{-1}

Glycolaldehyde #01 cation (C_1)

O	–1.321417	0.597486	0.176457
C	–0.059575	0.918359	–0.038775
H	–1.812700	0.355296	–0.626507
C	1.038962	–0.495502	0.058623
O	0.634232	–1.577856	0.117324
H	0.362529	1.481896	0.794557
H	0.220975	1.260443	–1.038753
H	2.079147	–0.121421	0.046908

E = –228.7783297
E[CCSD(T)/CBS] = –228.4398472
ZPVE = 153.9289 kJ mol^{-1}

Glycolaldehyde #01 (C_s)

O	–1.347777	0.557051	0.000000
C	0.000000	0.928681	0.000000

H	–1.361244	–0.412024	0.000000
C	0.924487	–0.257086	0.000000
O	0.512154	–1.390532	0.000000
H	0.245610	1.542549	0.878739
H	0.245610	1.542549	–0.878739
H	2.008081	–0.034791	0.000000

E = –229.1364389
E[CCSD(T)/CBS] = –228.8117491
ZPVE = 160.0387 kJ mol^{-1}

Glycolaldehyde #02 cation (C_1)

O	–1.293701	0.875070	–0.318733
C	–0.004669	1.079178	–0.123125
H	–1.818781	0.835904	0.498367
C	0.916406	–0.448994	0.059514
O	0.384232	–1.469662	0.177093
H	0.304852	1.555993	0.810961
H	0.490839	1.434410	–1.027793
H	1.994100	–0.203714	0.037714

E = –228.7783296
E[CCSD(T)/CBS] = –228.4398495
ZPVE = 153.9255 kJ mol^{-1}

Glycolaldehyde #02 (C_s)

O	1.302044	–0.690422	0.000000
C	0.770533	0.608140	0.000000
H	2.260995	–0.632407	0.000000
C	–0.737108	0.581953	0.000000
O	–1.420138	–0.402999	0.000000
H	1.072266	1.196088	–0.881008
H	1.072266	1.196088	0.881008
H	–1.182560	1.601071	0.000000

E = –229.1279011
E[CCSD(T)/CBS] = –228.8033010
ZPVE = 158.4770 kJ mol^{-1}

Glycolaldehyde #03 cation (C_1)

O	–1.285865	1.187448	–0.069553

C	0.010770	0.894365	–0.159239
H	–1.545293	1.528885	0.802634
C	0.201593	–0.844154	0.038605
O	1.118210	–1.232569	0.635639
H	0.680692	1.312135	0.588772
H	0.367322	0.942560	–1.192128
H	–0.606998	–1.397301	–0.468937

E = –228.7795703
E[CCSD(T)/CBS] = –228.4407168
ZPVE = 154.8563 kJ mol^{-1}

Glycolaldehyde #03 (C_s)

O	1.266366	1.879953	0.000000
C	0.780852	0.549904	0.000000
H	2.226566	1.866725	0.000000
C	–0.732015	0.603212	0.000000
O	–1.429426	–0.375206	0.000000
H	1.097250	–0.014804	0.885128
H	1.097250	–0.014804	–0.885128
H	–1.149033	1.630316	0.000000

E = –229.1305150
E[CCSD(T)/CBS] = –228.8061648
ZPVE = 158.0194 kJ mol^{-1}

Glycolaldehyde #04 cation (C_1)

O	–1.655967	–0.296531	0.091481
C	–0.632308	0.541599	–0.065199
H	–1.957754	–0.369893	1.012429
C	0.849516	–0.404311	–0.165399
O	1.804924	0.014665	0.343493
H	–0.428314	1.251992	0.732655
H	–0.590662	0.946389	–1.080413
H	0.696324	–1.329874	–0.746137

E = –228.7795703
E[CCSD(T)/CBS] = –228.4407254
ZPVE = 154.8491 kJ mol^{-1}

Glycolaldehyde #04 (C_1)

O	1.711792	0.231131	–0.003969
C	0.516542	–0.524498	–0.070449
H	1.807441	0.591696	0.882358
C	–0.727479	0.344174	–0.124089
O	–1.834586	–0.051751	0.125366
H	0.414279	–1.246715	0.745132
H	0.557408	–1.092706	–1.003885
H	–0.531156	1.394632	–0.427554

E = –229.1306407
E[CCSD(T)/CBS] = –228.8058664
ZPVE = 158.7039 kJ mol^{-1}

(*E*)-*trans, trans* Ethene-1,2-diol cation (C_{2h})

C	0.565043	–0.411377	0.000000
C	–0.565043	0.411377	0.000000
O	–1.728648	–0.167757	0.000000
H	–2.474330	0.455484	0.000000
H	–0.474010	1.492952	0.000000
O	1.728648	0.167757	0.000000
H	2.474330	–0.455484	0.000000
H	0.474010	–1.492952	0.000000

E = –228.8308768
E[CCSD(T)/CBS] = –228.4927525
ZPVE = 164.3151 kJ mol^{-1}

(*E*)-*trans, trans* Ethene-1,2-diol (C_2)

C	0.546618	0.375520	–0.072170
C	–0.546618	–0.375520	–0.072170
O	–1.795742	0.198153	0.014140
H	–2.440056	–0.395353	–0.379217
H	–0.486695	–1.457749	–0.069631
O	1.795742	–0.198153	0.014140
H	2.440056	0.395353	–0.379217
H	0.486695	1.457749	–0.069631

E = –229.1164359
E[CCSD(T)/CBS] = –228.7906112
ZPVE = 158.9087 kJ mol^{-1}

(*E*)-*cis, trans* Ethene-1,2-diol cation (C_s)

C	0.562695	–0.386979	0.000000
C	–0.575731	0.426942	0.000000
O	–1.730729	–0.173486	0.000000
H	–2.490323	0.432925	0.000000
H	–0.521130	1.511932	0.000000
O	1.782069	0.049292	0.000000
H	1.882148	1.017626	0.000000
H	0.469731	–1.467265	0.000000

E = –228.8258146
E[CCSD(T)/CBS] = –228.4878997
ZPVE = 164.1639 kJ mol^{-1}

(*E*)-*cis, trans* Ethene-1,2-diol (C_1)

C	0.536830	–0.375622	0.035089
C	–0.537963	0.404615	0.015759
O	–1.805363	–0.140589	–0.053859
H	–2.377261	0.305180	0.577977
H	–0.464535	1.488776	–0.026431
O	1.837491	0.041868	–0.013468
H	1.867842	1.003075	–0.071255
H	0.452875	–1.452261	0.071581

E = –229.1171363
E[CCSD(T)/CBS] = –228.7913099
ZPVE = 159.8009 kJ mol^{-1}

(*E*)-*cis, cis* Ethene-1,2-diol cation (C_2)

C	0.565367	0.412826	0.000000
C	–0.565367	–0.412826	0.000000
O	–0.524446	–1.709114	0.000000
H	0.367752	–2.099730	0.000000
H	–1.573260	–0.010024	0.000000
O	0.524446	1.709114	0.000000
H	–0.367752	2.099730	0.000000
H	1.573260	0.010024	0.000000

E = –228.8220855
E[CCSD(T)/CBS] = –228.4842479
ZPVE = 164.2288 kJ mol^{-1}

(*E*)-*cis, cis* Ethene-1,2-diol (C_2)

C	0.535588	–0.393538	0.000000
C	–0.535588	0.393538	0.000000
O	–0.531842	1.767126	0.000000
H	0.376318	2.087396	–0.000001
H	–1.544782	0.001982	0.000000
O	0.531842	–1.767126	0.000000
H	–0.376318	–2.087396	–0.000001
H	1.544782	–0.001982	0.000000

E = –229.1179891
E[CCSD(T)/CBS] = –228.7918952
ZPVE = 160.0722 kJ mol^{-1}

(*Z*)-*trans, trans* Ethene-1,2-diol cation (C_{2v})

C	0.000000	0.701558	0.598805
C	0.000000	–0.701558	0.598805
O	0.000000	–1.332423	–0.533871
H	0.000000	–2.299833	–0.440901
H	0.000000	–1.241982	1.538413
O	0.000000	1.332423	–0.533871
H	0.000000	2.299833	–0.440901
H	0.000000	1.241982	1.538413

E = –228.8302182
E[CCSD(T)/CBS] = –228.4928958
ZPVE = 165.1683 kJ mol^{-1}

(*Z*)-*trans, trans* Ethene-1,2-diol (C_{2v})

C	0.000000	0.664463	0.621475
C	0.000000	–0.664463	0.621475
O	0.000000	–1.402610	–0.534851
H	0.000000	–2.335599	–0.311700
H	0.000000	–1.196227	1.562811
O	0.000000	1.402610	–0.534851
H	0.000000	2.335599	–0.311700
H	0.000000	1.196227	1.562811

E = –229.1175585
E[CCSD(T)/CBS] = –228.7924957
ZPVE = 159.4846 kJ mol^{-1}

(*Z*)-*cis, trans* Ethene-1,2-diol cation (C_s)

C	–0.702451	0.603136	0.000000
C	0.700873	0.624098	0.000000
O	1.320059	–0.524193	0.000000
H	2.289374	–0.455608	0.000000
H	1.249525	1.558079	0.000000
O	–1.406398	–0.480047	0.000000
H	–0.876304	–1.299567	0.000000
H	–1.273536	1.522636	0.000000

E = –228.8297013
E[CCSD(T)/CBS] = –228.4931010
ZPVE = 165.1353 kJ mol^{-1}

(*Z*)-*cis, trans* Ethene-1,2-diol (C_1)

C	–0.677832	0.628855	–0.006113
C	0.650200	0.655746	0.024604
O	1.350196	–0.541555	–0.008760
H	2.136784	–0.472167	0.538569
H	1.212465	1.578185	0.006253
O	–1.425013	–0.509633	–0.006957
H	–0.814926	–1.257861	0.033254
H	–1.268115	1.530816	–0.049918

E = –229.1242472
E[CCSD(T)/CBS] = –228.7993516
ZPVE = 161.5028 kJ mol^{-1}

Methyl formate #01 cation (C_s)

C	–0.322049	–0.641116	0.000000
O	0.023000	0.561966	0.000000
C	1.463697	0.969181	0.000000
H	1.582746	1.563796	0.898772
H	1.582746	1.563796	–0.898772
H	2.091024	0.082431	0.000000
O	–1.520570	–1.027292	0.000000
H	0.385178	–1.493543	0.000000

E = –228.7632192
E[CCSD(T)/CBS] = –228.4253033
ZPVE = 156.7613 kJ mol^{-1}

Methyl formate #01 (C_s)

C	–0.357854	–0.676644	0.000000
O	0.000000	0.620530	0.000000
C	1.393737	0.939881	0.000000
H	1.613905	1.526903	0.889587
H	1.613905	1.526903	–0.889587
H	2.008234	0.037411	0.000000
O	–1.495027	–1.034159	0.000000
H	0.508874	–1.361607	0.000000

E = –229.1489027
E[CCSD(T)/CBS] = –228.8193960
ZPVE = 160.5394 kJ mol^{-1}

Methyl formate #02 cation (C_s)

C	–0.726324	0.499868	0.000000
O	0.517087	0.671541	0.000000
C	1.461909	–0.498483	0.000000
H	1.279460	–1.069809	0.905805
H	2.438191	–0.031936	0.000000
H	1.279460	–1.069809	–0.905805
O	–1.329742	–0.607297	0.000000
H	–1.391519	1.380858	0.000000

E = –228.7649376
E[CCSD(T)/CBS] = –228.4277752
ZPVE = 156.8178 kJ mol^{-1}

Methyl formate #02 (C_s)

C	–0.763903	0.440753	0.000000
O	0.548851	0.702755	0.000000
C	1.416163	–0.447709	0.000000
H	1.241385	–1.054217	0.886666
H	2.426459	–0.051730	0.000000
H	1.241385	–1.054217	–0.886666
O	–1.264527	–0.648895	0.000000
H	–1.317291	1.388190	0.000000

E = –229.1561630
E[CCSD(T)/CBS] = –228.8279453

ZPVE = 162.2987 kJ mol^{-1}

1,3-Dioxetane cation (D_{2h})

O	–0.000000	1.027455	–0.000000
C	–0.959569	–0.000000	–0.000000
C	0.959569	0.000000	–0.000000
O	0.000000	–1.027455	–0.000000
H	1.601708	0.000000	0.901513
H	1.601708	0.000000	–0.901513
H	–1.601708	–0.000000	–0.901513
H	–1.601708	–0.000000	0.901513

E = –228.7351245
E[CCSD(T)/CBS] = –228.3940852
ZPVE = 154.0980 kJ mol^{-1}

1,3-Dioxetane (D_{2h})

O	0.000000	0.000000	–1.035573
C	0.000000	–0.983257	–0.000000
C	–0.000000	0.983257	0.000000
O	0.000000	–0.000000	1.035573
H	–0.901963	1.605219	0.000000
H	0.901963	1.605219	0.000000
H	0.901963	–1.605219	–0.000000
H	–0.901963	–1.605219	–0.000000

E = –229.0928022
E[CCSD(T)/CBS] = –228.7688123
ZPVE = 164.9067 kJ mol^{-1}

Oxiran-2-ol cation (C_s)

O	0.527608	0.342942	–0.000000
C	–0.498017	–0.418009	0.000000
C	1.818337	–0.083049	–0.000000
H	2.532888	0.720249	–0.000000
H	2.021937	–1.143049	0.000000
O	–1.629146	0.180763	0.000000
H	–2.393248	–0.420867	0.000000
H	–0.400214	–1.501904	0.000000

E = –228.7891396

E[CCSD(T)/CBS] = –228.4507662
ZPVE = 156.2551 kJ mol^{-1}

Oxiran-2-ol (C_1)

O	0.761180	–0.801134	–0.253427
C	–0.212023	–0.048313	0.449567
C	0.993220	0.605920	–0.031809
H	0.913143	1.224709	–0.918238
H	1.803114	0.843711	0.649107
O	–1.397976	0.230345	–0.200034
H	–1.992184	–0.521689	–0.105163
H	–0.316887	–0.326062	1.495432

E = –229.1048487
E[CCSD(T)/CBS] = –228.7812503
ZPVE = 162.5001 kJ mol^{-1}

Notes and References

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