Supporting information for: "Energetic and Spectroscopic Insights into the $C_3H_6O_2$ Isomer Family for Astrochemical Purposes"

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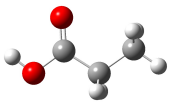
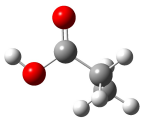
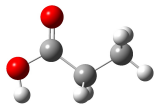
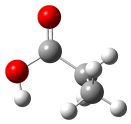
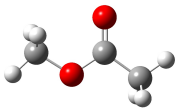
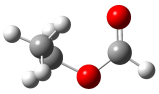
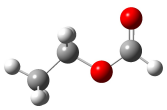
Table S1: Elapsed time [a] for each step of the protocol for 2-hydroxypropanal (**2a**) and `inner` glycidol.

Elapsed time		**Unit**	**Step**
2-hydroxypropanal (**2a**)	`inner` glycidol		
8	8	seconds	1-2
5	1	hours	3
27	91	days	4

[a] Calculations performed on an AMD EPYC 7282 16-Core Processor CPU, on nodes with 256 GB of RAM.

Table S2: Label, structure, and relative energy (with and without hZPE correction) for the $C_3H_6O_2$ species considered in the preliminary investigations (Steps 1 and 2 of the protocol).

LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
2a		propanoic acid	0	0
2c			4.91	5.50
2b			22.49	21.79
2d			28.46	28.14
3a		methyl acetate	39.40	36.65
4b		ethyl formate	55.08	55.32
4a			56.04	55.45

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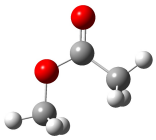
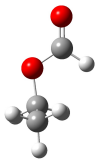
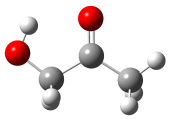
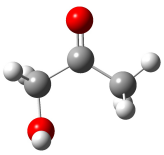
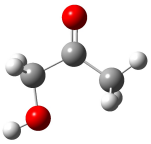
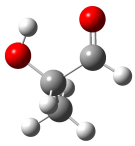
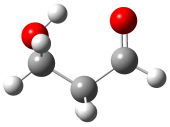
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
3b			69.23	66.52
4c			73.69	72.07
5a		1-hydroxyacetone	87.43	83.38
5c			103.96	99.60
5d			105.09	99.98
6d		2-hydroxypropanal	106.49	103.15
1c		3-hydroxypropanal	112.92	112.12

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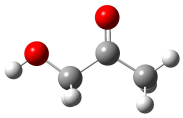
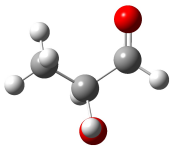
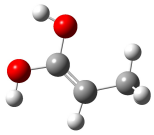
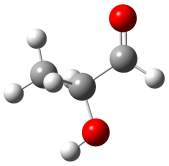
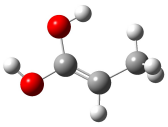
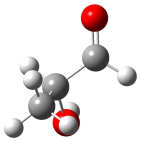
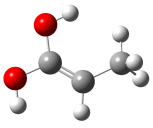
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
5b			117.70	112.28
6b			119.18	114.92
18b		1-propene-1,1-diol	119.95	115.89
6a			121.50	116.48
18c			122.00	117.36
6c			122.52	118.01
18d			125.62	122.17

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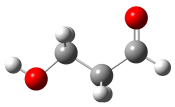
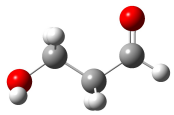
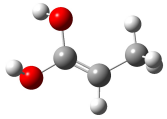
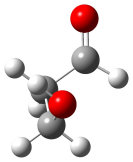
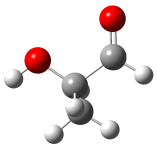
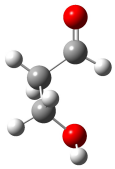
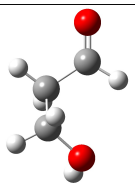
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
1a			127.33	124.39
1b			128.21	125.41
18a			129.68	126.41
1h			129.69	127.07
6e			132.83	128.07
1i			132.02	129.00
1l			131.76	129.22

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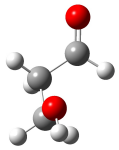
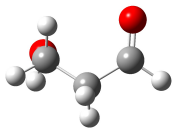
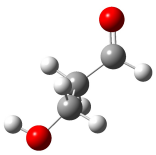
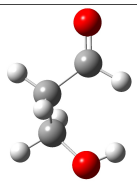
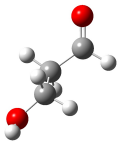
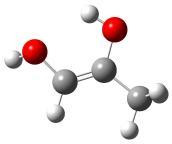
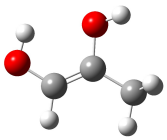
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
1g			132.51	129.28
1d			133.08	130.08
1f			133.71	131.33
1m			134.85	131.75
1e			136.57	133.35
14a		(1Z)-propene-1,2-diol	136.41	133.98
14b			138.88	136.49

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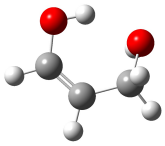
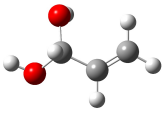
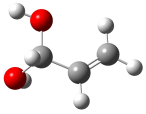
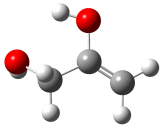
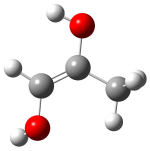
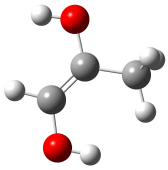
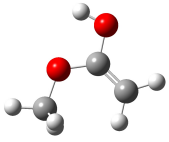
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
11b		(1Z)-propene-1,3-diol	145.28	147.90
16d		2-propene-1,1-diol	149.16	148.27
16e			149.09	148.28
12c		2-propene-1,2-diol	149.01	149.48
15b		(1E)-propene-1,2-diol	153.68	149.62
15d			154.01	149.83
13a		1-methoxy eth-1-enol	154.52	152.04

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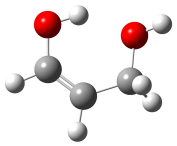
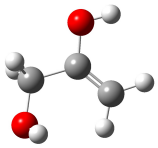
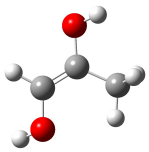
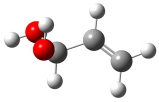
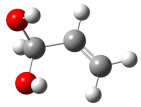
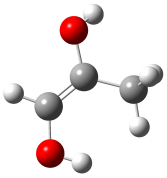
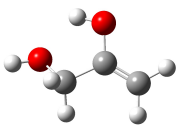
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
11e			151.25	152.32
12f			154.31	153.14
15a			158.24	153.27
16a			155.89	153.85
16f			155.92	154.71
15c			158.87	154.75
12d			155.85	155.15

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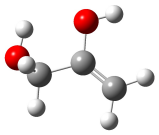
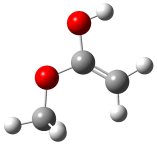
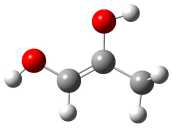
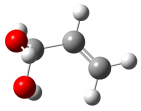
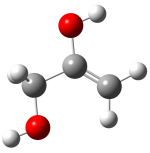
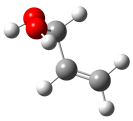
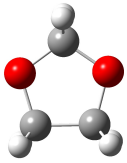
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
12h			156.80	155.56
13d			159.88	157.89
14c			163.47	157.93
16h			161.33	159.61
12e			162.51	159.77
16b			163.28	160.33
25a		1,3-dioxolane	155.27	161.09

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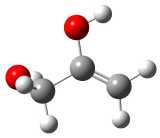
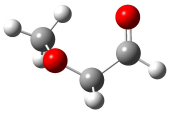
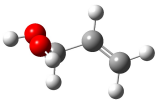
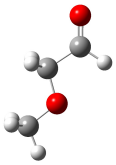
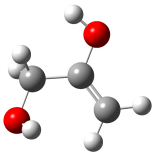
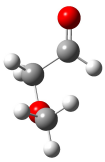
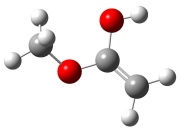
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
12g			162.58	161.27
7b		methoxyacetaldehyde	165.63	161.39
16c			164.71	161.47
7c			167.39	161.54
12b			163.61	161.58
7d			167.25	162.66
13b			167.06	163.61

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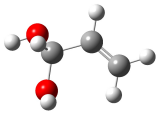
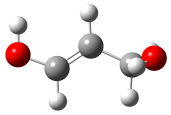
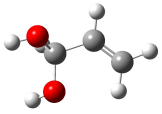
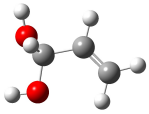
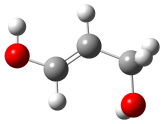
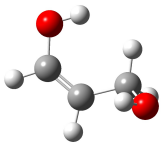
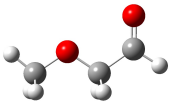
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
16l			167.02	164.31
10h		(1E)-propene-1,3-diol	164.86	164.74
16g			167.88	164.81
16i			169.94	166.24
10f			167.55	167.59
11g			167.91	168.02
7a			173.53	168.45

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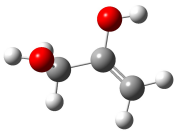
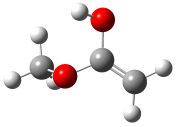
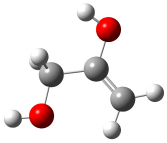
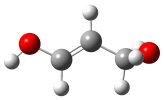
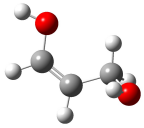
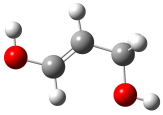
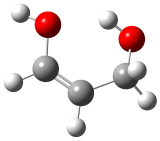
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
12i			171.14	168.45
13c			172.66	169.16
12a			174.77	170.58
10c			173.82	172.56
11c			173.14	172.57
10e			174.20	172.71
11a			173.68	173.01

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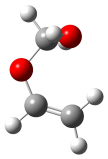
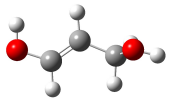
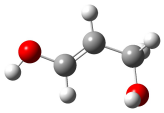
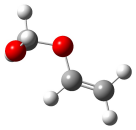
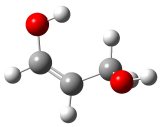
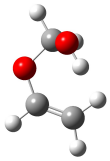
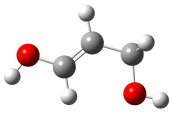
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
19f		ethenyloxy methanol	172.91	173.03
10g			174.42	173.13
10b			174.63	173.68
19b			176.14	174.80
11f			176.89	176.00
19e			176.32	176.65
10a			180.32	177.91

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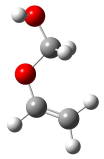
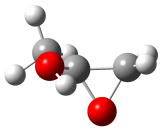
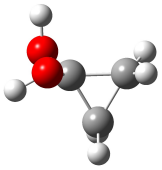
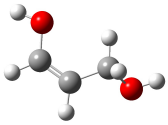
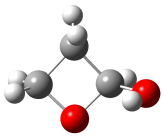
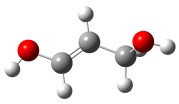
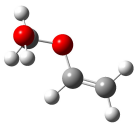
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
19d			179.37	178.85
36b		glycidol	182.41	179.29
32a		cyclopropane-1,1-diol	180.27	179.31
11d			181.87	179.95
29a		oxetan-2-ol	177.86	180.85
10d			183.70	181.24
19c			183.87	182.11

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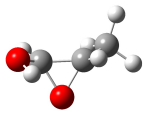
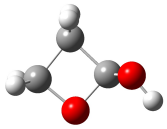
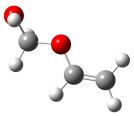
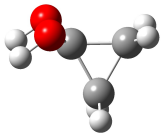
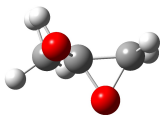
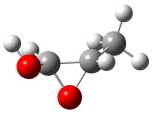
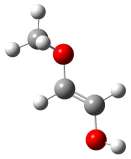
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
34b		3-methyl-oxiran-2-ol	185.83	183.68
29b			181.66	184.27
19a			187.66	185.15
32b			191.82	189.78
36a			194.09	190.39
34a			198.20	194.53
22		(E)-2-methoxy ethenol	212.69	208.38

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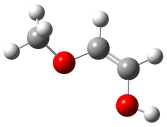
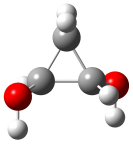
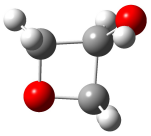
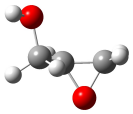
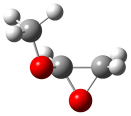
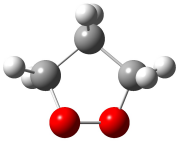
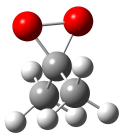
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
23		(Z)-2-methoxy ethenol	213.55	209.92
35		cyclopropane-1,2-diol	221.65	220.18
27		oxetan-3-ol	219.00	220.80
30		2-oxiranylmethanol	237.52	236.82
33		2-methoxyoxirane	249.04	247.06
26		1,2-dioxacyclopentane	343.74	346.75
31		3,3-dimethyldioxirane	354.31	347.63

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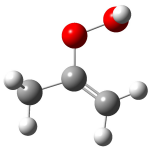
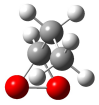
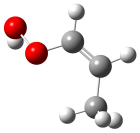
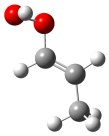
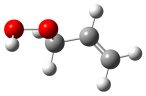
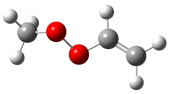
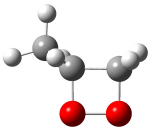
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
17		2-hydroperoxyprop-1-ene	370.49	362.69
38		ethyl dioxirane	380.59	377.19
21		1-hydroperoxy-(1Z)-propene	388.08	380.60
20		1-hydroperoxy-(1E)-propene	389.79	381.57
9		3-hydroperoxyprop-1-ene	410.33	403.36
24		methylperoxy ethene	412.64	404.25
28		3-methyl-1,2-dioxetane	416.71	414.63

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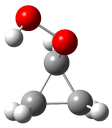
LABEL	STRUCTURE	NAME	E_{el} [a]	E_{el}+hZPE [a]
37		1-hydroperoxy cyclopropane	431.87	426.62

[a] The electronic energy E_{el} and the hZPE correction are computed at the B3LYP/cc-pVDZ level of theory. The energy of **2a** is taken as reference (equilibrium energy = -268.4277894 E_h and hZPE correction = 0.0900259 E_h). The values reported are in kJ/mol.

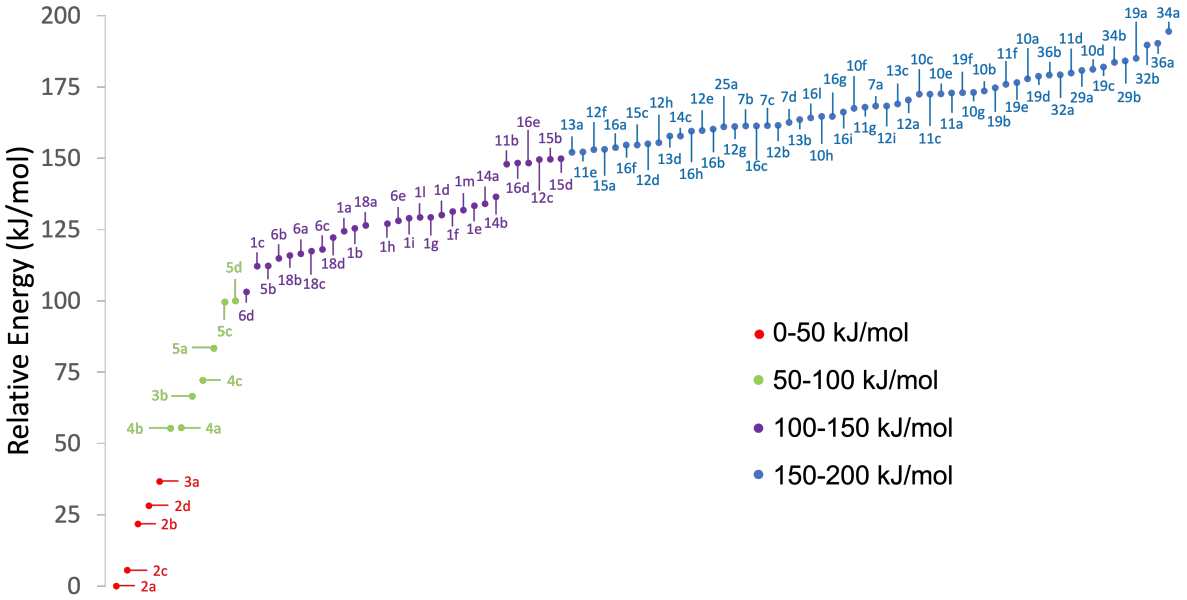


Figure S1: B3LYP/cc-pVDZ hZPE-corrected relative energies of the 97 $C_3H_6O_2$ conformers considered in Step 2. The energy of **2a** is taken as reference (equilibrium energy = -268.427789 E_h and hZPE correction = 0.090026 E_h).

Table S3: Relative energy (with and without hZPE correction) and total electric dipole moment (debye) for the $C_3H_6O_2$ conformers considered in Step 3 of the protocol.

ISOMER	$\mathbf{E_{el}}$ [a]	$\mathbf{E_{el}}$**+hZPE** [a]	**Total Dipole Moment** [b]
2a	0	0	1.57
2c	3.59	4.32	1.81
2b	20.25	19.77	4.22
2d	25.50	25.42	4.44
3a	41.53	39.71	1.83
4a	57.91	58.01	2.13
4b	58.60	59.26	1.92
3b	72.00	70.01	4.55
4c	77.21	76.03	4.42
5a	83.02	79.59	3.22
5d	97.80	93.49	2.81
5c	99.54	95.54	2.12
6d	101.51	98.47	2.60
5b	108.39	103.56	4.36
1c	109.71	108.88	3.02
6a	114.00	109.19	2.89
6c	113.51	109.47	1.49
6b	114.78	110.42	1.56
18b	114.82	111.19	1.31
18c	117.34	113.10	1.66
1a	118.45	115.92	1.25
1g	121.25	118.51	4.36
1h	121.04	118.61	3.13

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ISOMER	E_{el} [a]	E_{el}+hZPE [a]	Total Dipole Moment [b]
18d	121.65	118.61	2.22
1b	121.71	118.99	2.83
6e	124.20	119.70	4.32
1i	122.05	119.71	4.44
18a	124.46	121.23	1.31
1l	124.52	121.99	3.35
1e	124.64	122.10	3.02
1f	124.67	122.46	1.33
1d	125.70	123.00	4.11
14a	114.82	125.32	2.06
14b	130.89	128.18	2.75
16e	136.07	135.06	0.20
16d	136.28	135.21	0.15
12c	141.26	141.02	1.65
15b	147.34	143.27	1.96
15d	147.34	144.75	0.51
11b	144.54	146.70	2.05

[a] The electronic energy E_{el} and the hZPE correction are computed at the revDSDPBEP86/jun-cc-pVTZ level of theory. The energy of **2a** is taken as reference (electronic energy = -268.0460105 E_h and hZPE correction = 0.0908268 E_h). The values reported are in kJ/mol.

[b] The total dipole moment is computed at the revDSDPBEP86/jun-cc-pVTZ level of theory. The values reported are in debye.

Table S4: Experimental spectroscopic parameters (A-reduction) of the `inner` and `outer` conformers of glycidol.

		`inner`		`outer`	
Constant	Unit	This work[a]	Marstokk et al.[1]	This work[a]	Marstokk et al.[1]
A_0	MHz	10347.8659(1)	10347.8575(1)	13857.0862(2)	13857.0779(4)
B_0	MHz	4102.36084(4)	4102.35728(4)	3420.50500(5)	3420.50399(9)
C_0	MHz	3781.95191(4)	3781.94826(4)	3065.87772(5)	3065.8781(1)
Δ_J	kHz	2.38385(2)	2.38257(5)	2.33346(3)	2.3412(3)
Δ_{JK}	kHz	-1.43220(8)	-1.4269(3)	-15.2339(2)	-15.156(3)
Δ_K	kHz	5.1842(3)	5.1812(1)	54.8963(8)	54.852(2)
δ_J	kHz	0.314837(7)	0.315582(9)	0.40322(1)	0.40240(9)
δ_K	kHz	-9.7037(2)	-9.782(1)	3.3009(6)	3.184(8)
Φ_J	mHz	-2.175(5)	-4.03(2)	5.467(8)	10.532(3)
Φ_{JK}	mHz	11.26(6)	16.60(2)	-62.0(1)	-
Φ_{KJ}	mHz	-30.6(2)	-104.4(4)	118.5(5)	237.4(2)
Φ_K	mHz	39.2(4)	77.2(2)	122.7(8)	-
ϕ_J	mHz	-0.300(2)	-	1.407(3)	-
ϕ_{JK}	mHz	69.16(4)	-	-23.9(3)	-
ϕ_K	mHz	-438.(2)	-	438.(3)	-
Λ_J	µHz	-0.0044(4)	-	0.0232(7)	-
Λ_{JJK}	µHz	0.376(2)	-	-0.386(7)	-
Λ_{JK}	µHz	-4.72(1)	-	-1.81(7)	-
Λ_{KKJ}	µHz	10.93(5)	-	-2.5(3)	-
Λ_K	µHz	-6.5(1)	-	-	-
λ_J	µHz	0.0017(1)	-	0.0078(3)	-
λ_{JK}	µHz	-	-	0.36(3)	-
Lines[b]		3748/5932		2795/4853	
Max. J, K_a		99, 46		89, 39	
rms	kHz	39.5		39.9	
St. Dev.		0.98		1.04	

[a] The standard errors as provided by `PIFORM` (Z. Kisiel, PROSPE - Programs for ROtational SPEctroscopy, `http://info.ifpan.edu.pl/~kisiel/prospe.htm`) are indicated in parentheses. Experimental dipole moment values are from Marstokk et al.[1].
[b] Distinct frequencies included in the fit / Total number of transitions. Our dataset includes 73 transitions for `inner` and 66 for `outer` from Marstokk et al.[1].

Table S5: Comparison between computed [a] and experimental [b] quartic and sextic centrifugal distortion constants for `inner` and `outer` glycidol, *trans* and *gauche* ethyl formate, and 2- and 3-hydroxypropanal.

Constant	**Unit**	**`inner` glycidol**		**`outer` glycidol**		**2-hydroxypropanal**	
		Exp.[c]	Theo.	Exp.[c]	Theo	Exp.[d]	Theo
D_J / Δ_J	kHz	2.50514(1)	2.54	2.30591(3)	2.30	1.784714(65)	1.79
D_K / Δ_K	kHz	5.7911(2)	5.79	54.7590(8)	53.83	17.82873(73)	18.54
D_{JK} / Δ_{JK}	kHz	-2.16004(7)	-2.35	-15.0687(2)	-15.05	-2.09014(21)	-2.41
d_1 / δ_J	kHz	-0.314786(3)	-0.325	-0.403240(10)	-0.40	0.304926(10)	0.31
d_2 / δ_K	kHz	0.060684(1)	0.056	-0.013772(3)	-0.01	2.57516(14)	2.47
H_J / Φ_J	Hz	$-2.537(1)\times10^{-3}$	-2.8×10^{-3}	$5.498(8)\times10^{-3}$	6.9×10^{-3}	0.004466(23)	0.0047
H_K / Φ_K	Hz	$24.0(1)\times10^{-3}$	26.6×10^{-3}	0.0964(8)	0.065	0.1122(10)	0.087
H_{JK} / Φ_{JK}	Hz	$7.11(2)\times10^{-3}$	8.7×10^{-3}	-0.07388(7)	-0.091	-0.00694(10)	-0.0096
H_{KJ} / Φ_{KJ}	Hz	$-11.02(8)\times10^{-3}$	-14.8×10^{-3}	0.1576(4)	0.2368	-0.9838(52)	-0.087
h_1 / ϕ_J	mHz	-0.2984(3)	-0.383	1.395(3)	1.85	0.8170(20)	0.93
h_2 / ϕ_{JK}	mHz	0.1607	0.139	-0.017(1)	-0.013	8.712(46)	8.90
h_3 / ϕ_K	mHz	0.01296(7)	0.009	0.01155(7)	0.012	5.61(23)	3.97
μ_a	D	0.61(2)	0.63	1.25(6)	1.31		
μ_b	D	1.20(9)	1.23	1.650(1)	1.51		
μ_c	D	0.51(12)	0.78	0.154(2)	0.19		
Constant	**Unit**	***trans* ethyl formate**		***gauche* ethyl formate**		**3-hydroxypropanal**	
		Exp.[d]	Theo	Exp.[d]	Theo	Exp.[d]	Theo
D_J / Δ_J	kHz	0.6243410(238)	0.622	5.93910(91)	5.61	4.010060(69)	3.84
D_K / Δ_K	kHz	51.3539(120)	48.7	78.7548(167)	-69.3	12.99819(71)	11.5
D_{JK} / Δ_{JK}	kHz	-3.48608(285)	-3.60	-32.3373(38)	-29.40	-9.53279(46)	-8.58
d_1 / δ_J	kHz	0.1017021(129)	0.104	2.00186(36)	1.87	1.274532(30)	1.21
d_2 / δ_K	kHz	-0.9852(33)	-0.634	7.1777(187)	6.62	5.30738(43)	5.04
H_J / Φ_J	Hz	-	5.37×10^{-5}	-0.05934(40)	-0.052	-0.019624(13)	-0.016
H_K / Φ_K	Hz	-	1.19	7.650(43)	5.46	0.25706(76)	0.21
H_{JK} / Φ_{JK}	Hz	-	0.307×10^{-3}	0.9168(39)	0.67	0.12908(25)	0.11
H_{KJ} / Φ_{KJ}	Hz	-0.8331(174)	-0.737	-4.1566(119)	-3.05	-0.28906(53)	-0.26
h_1 / ϕ_J	mHz	-	0.029	-25.608(175)	-22.5	-9.1793(59)	-7.55
h_2 / ϕ_{JK}	mHz	-24.11(103)	-4.71	-73.4(112)	-127.7	-61.90(11)	-43.7
h_3 / ϕ_K	mHz	-209.(43)	-210.6	1785.(42)	548.7	-81.47(63)	-50.1
μ_a	D	1.85(2)	1.94	1.44(6)	1.55		
μ_b	D	0.69(8)	0.74	1.05(3)	1.05		
μ_c	D	0[e]	0.0	0.25	0.25		

[a] Computed at the revDSD/junTZ level of theory. [b] The experimental references are taken from this work for glycidol, from ref. 2 for 2-hydroxypropanal, ref. 3 for both isomers of ethyl formate and ref. 4 for 3-hydroxypropanal. [c] Watson's S reduction. [d] Watson's A reduction. [e] Assumed in ref. 5.

Table S6: Computed vibrational ground state rotational constants, [a] quartic and sextic centrifugal distortion terms, [b] and electric dipole moment [b] of the most stable $C_3H_6O_2$ species without experimental spectroscopic characterization (**2c**, **2b**, **2d**, **3b**, **4c**, **5d**, **5c**, and **5b**).

Constant	**Unit**	**2c**	**2b**	**2d**	**3b**	**4c**	**5d**	**5c**	**5b**
A_0	MHz	8765.46	10001.51	8596.98	8998.87	17316.55	8618.53	8521.05	9948.93
B_0	MHz	3944.39	3830.59	3944.63	4391.62	2658.67	4087.15	4006.09	3728.44
C_0	MHz	3135.87	2869.75	3102.28	3065.45	2535.42	2878.21	2858.11	2808.87
D_J	kHz	2.15	0.727	1.938	0.625	2.95	0.694	0.774	0.652
D_K	kHz	−132.1	2.81	−116.2	−0.170	814.7	−0.171	−0.703	6.54
D_{JK}	kHz	164.1	3.45	145.1	5.25	−70.9	5.20	7.39	3.84
d_1	kHz	0.202	−0.193	−0.0175	−0.208	−0.830	−0.233	−0.181	−0.173
d_2	kHz	−0.0375	−0.0192	−0.0164	−0.0485	−0.0407	−0.0643	−0.106	−0.0268
H_J	mHz	−86.5	0.335	−76.7	−0.0686	−33.5	0.541	0.902	−0.0407
H_K	Hz	12.4	0.0223	11.6	−0.00113	372.9	−0.0182	0.276	0.0381
H_{JK}	mHz	1373.0	−19.6	1316.0	−5.12	1517.7	−25.3	4.40	−5.14
H_{KJ}	Hz	−7.22	0.0125	−7.646	0.00983	−36.9	0.0506	−0.356	−0.0145
h_1	mHz	11.9	0.0607	11.4	0.0601	−12.3	−0.0444	−0.517	0.0673
h_2	mHz	25.8	−0.122	22.9	0.0211	0.314	−0.308	0.102	0.101
h_3	mHz	6.22	0.000747	5.11	−0.0540	0.101	0.0403	−0.121	−0.00450
$\lvert\mu_a\rvert$	D	1.26	1.68	3.78	3.22	3.97	2.80	1.57	0.08
$\lvert\mu_b\rvert$	D	1.26	3.87	1.90	3.22	0.23	0.14	1.11	4.36
$\lvert\mu_c\rvert$	D	0.33	0.00	1.36	0.00	1.91	0.00	0.89	0.14
μ_{tot}	D	1.81	4.22	4.44	4.55	4.42	2.81	2.12	4.36

[a] CCSD(T)/CBS+CV equilibrium rotational constants augmented by revDSD/junTZ vibrational contributions. [b] Computed at the revDSD/junTZ level of theory.

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