

Supporting Information for

Mechanistical study on the formation of hydroxyacetone ($\text{CH}_3\text{COCH}_2\text{OH}$), methyl acetate ($\text{CH}_3\text{COOCH}_3$), and 3-hydroxypropanal ($\text{HCOCH}_2\text{CH}_2\text{OH}$) along with their enol tautomers (prop-1-ene-1,2-diol ($\text{CH}_3\text{C}(\text{OH})\text{CHOH}$), prop-2-ene-1,2-diol ($\text{CH}_2\text{C}(\text{OH})\text{CH}_2\text{OH}$), 1-methoxyethen-1-ol ($\text{CH}_3\text{OC}(\text{OH})\text{CH}_2$) and prop-1-ene-1,3-diol ($\text{HOCH}_2\text{CHCHOH}$)) in interstellar ice analogs

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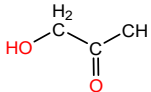
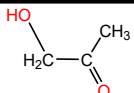
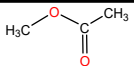
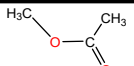
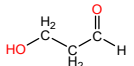
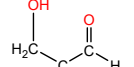
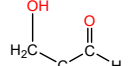
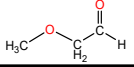
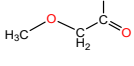
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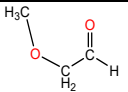
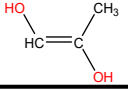
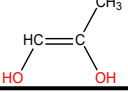
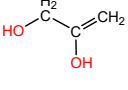
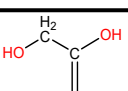
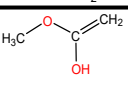
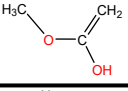
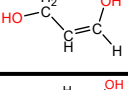
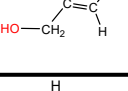
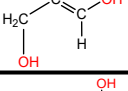
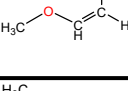
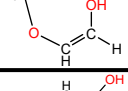
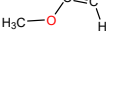
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Table S1. Error analysis of adiabatic ionization energies (IE) and relative energies (E_{rel}) of distinct $\text{C}_3\text{H}_6\text{O}_2$ isomers; IEs and E_{rel} were computed at the CCSD(T)-F12/CC-pVTZ-F12// ω B97X-D/cc-pVTZ level of theory including the zero-point vibrational energy corrections. Their computed Cartesian coordinates and vibrational frequencies are shown in Table S2.

Name	Isomer	Structure	E_{rel} (kJ mol ⁻¹)	Experimental IE (eV)	Computed IE (eV)	IE difference to lower bound (eV)	IE difference to upper bound (eV)	IE range after error analysis (eV)	Corrected IE with electric field effect (eV)
Hydroxyac etone	1a		39		9.60			9.52 – 9.68	9.49 – 9.65
	1b		53		10.08			10.00 – 10.16	9.97 – 10.13
Methyl acetate	2a		0	10.25 ± 0.05 ₁	10.27	-0.07	0.03	10.19 – 10.35	10.16 – 10.32
	2b		31		9.41			9.33 – 9.49	9.30 – 9.46
3- hydroxypro panal	3a		78		10.03			9.95 – 10.11	9.92 – 10.08
	3b		68	9.90 ± 0.05 ²	9.88	-0.03	0.07	9.80 – 9.96	9.77 – 9.93
	3c		82		10.11			10.03 – 10.19	10.00 – 10.16
2- methoxyac etaldehyde	4a		131		9.47			9.39 – 9.55	9.36 – 9.52
	4b		123		9.55			9.47 – 9.63	9.44 – 9.60

	4c		127	9.51	9.43 – 9.59	9.40 – 9.56
prop-1-ene-1,2-diol	5a		102	7.81	7.73 – 7.89	7.70 – 7.86
	5b		101	7.85	7.77 – 7.93	7.74 – 7.90
prop-2-ene-1,2-diol	6a		106	8.90	8.82 – 8.98	8.79 – 8.95
	6b		101	8.86	8.78 – 8.94	8.75 – 8.91
1-methoxyethen-1-ol	7a		123	8.13	8.05 – 8.21	8.02 – 8.18
	7b		116	8.42	8.34 – 8.50	8.31 – 8.47
prop-1-ene-1,3-diol	8a		117	8.78	8.70 – 8.86	8.67 – 8.83
	8b		120	8.89	8.81 – 8.97	8.78 – 8.94
	8c		120	8.57	8.49 – 8.65	8.46 – 8.62
2-methoxyethen-1-ol	9a		163	7.88	7.80 – 7.96	7.77 – 7.93
	9b		165	8.01	7.93 – 8.09	7.90 – 8.06
	9c		167	7.85	7.77 – 7.93	7.74 – 7.90

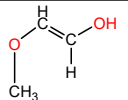
9d		163	8.03	7.95 – 8.11	7.92 – 8.08
			Average -0.05 ± 0.03	Average +0.05 ± 0.03	
			Combined error limits -0.08 – +0.08		

Table S2. Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) of neutral C₃H₆O₂ molecules (shown in Figure 2) as well as their respective monocations computed at the ωB97X-D/cc-pVTZ theory level.

Isomer	Vibration frequencies (cm ⁻¹)			Cartesian coordinates (Å)			
				Atom	X	Y	Z
1a				O	1.923732	-0.076789	-0.026575
	94.4637	136.2090	301.0849	C	0.721458	-0.771708	0.023641
	414.9140	424.9803	491.5268	C	-0.471189	0.162776	0.010883
	630.5218	822.1221	871.1799	C	-1.839411	-0.456274	-0.012366
	987.6416	1106.6050	1156.1980	O	-0.287257	1.356272	0.009979
	1224.2324	1272.3170	1333.2071	H	1.683742	0.858701	-0.014535
	1410.3897	1460.1763	1477.7245	H	0.653540	-1.384281	0.932737
	1483.2724	1497.5457	1829.8264	H	0.628527	-1.461188	-0.824740
	3004.0753	3034.4374	3060.0203	H	-2.595438	0.300574	0.175832
	3129.4864	3174.7052	3768.5339	H	-1.914576	-1.256596	0.724271
			H	-2.012740	-0.901834	-0.993751	
1a⁺				O	-1.947452	-0.047088	-0.266845
	53.9942	132.0517	226.4620	C	-0.921590	-0.707354	0.211640
	257.5249	356.7191	410.0558	C	0.651734	0.272764	0.029237
	493.6897	563.7727	859.2452	C	1.813196	-0.649977	-0.082409
	904.9423	1028.2806	1051.6044	O	0.491557	1.416648	0.038882
	1155.3179	1214.7028	1320.7059	H	-2.351043	0.556575	0.369728
	1376.5964	1406.1416	1442.6025	H	-0.655547	-1.557770	-0.410840
	1459.6626	1522.9662	2034.1208	H	-0.849983	-0.843406	1.292361
	3058.8810	3067.8286	3149.1734	H	2.721273	-0.082730	0.111606
	3181.8238	3192.6749	3804.2336	H	1.819619	-1.041255	-1.102190
			H	1.702798	-1.480494	0.612233	
1b				O	1.753876	0.296593	0.053975
	71.0699	143.9319	221.3558	C	0.791856	-0.727232	-0.048334
	267.2098	480.2743	505.0050	H	2.625785	-0.090143	-0.010455
	519.1578	773.6081	877.2936	H	0.870344	-1.456973	0.763632
	990.2226	1102.9486	1125.6325	H	0.873898	-1.274503	-0.994524
	1207.4991	1264.3880	1280.5690	C	-0.618144	-0.158377	-0.000582
	1399.5617	1439.7425	1466.3958	C	-0.774528	1.335183	-0.017645
	1466.5342	1499.6904	1839.7204	O	-1.551234	-0.919755	0.034630
	3021.4424	3065.9481	3068.4918	H	-1.830671	1.587718	0.004608
	3137.9511	3178.9983	3926.8632	H	-0.299639	1.748524	-0.908279
			H	-0.255962	1.773232	0.835537	
1b⁺				O	-1.788749	0.325985	-0.132450
	61.0310	106.2159	224.7380	C	-0.980262	-0.636973	0.282889
	287.3063	383.9959	454.6613	H	-2.159875	0.152014	-1.006280
	519.0423	565.7702	877.7412	H	-1.039975	-1.601158	-0.215041
	900.8322	1023.2735	1046.9213	H	-0.903248	-0.669516	1.370540
	1159.6282	1241.5619	1297.8170	C	0.732182	-0.158864	-0.002182
	1373.2427	1392.4877	1438.2443	C	0.932409	1.314820	0.058144
	1452.0603	1516.4891	1987.0285	O	1.427919	-1.072639	-0.164337
	3065.8483	3077.0634	3152.1547	H	1.998822	1.523227	0.030677
	3190.2786	3193.9398	3810.2911	H	0.464155	1.702703	0.961970
			H	0.420779	1.752058	-0.800672	

2a	84.8082	151.1990	177.4381	C	1.860090	-0.161213	-0.006254
	288.5871	434.6598	622.0374	O	0.547129	-0.715181	0.010198
	655.2598	878.4947	1007.3458	C	-0.456774	0.174682	0.006867
	1081.5626	1105.1944	1182.3983	C	-1.790823	-0.515059	-0.002782
	1214.5710	1305.5818	1418.9417	O	-0.286395	1.363230	0.001015
	1477.9026	1486.7541	1492.1968	H	2.018940	0.477765	0.860891
	1494.3425	1497.4243	1845.7077	H	2.016756	0.426578	-0.909502
	3071.1502	3078.5091	3148.6650	H	2.540557	-1.006914	0.016282
	3151.9216	3180.2273	3189.3541	H	-2.577049	0.219055	0.139636
				H	-1.830987	-1.274051	0.776117
			H	-1.929050	-1.017295	-0.960116	
2a⁺				C	-1.932769	-0.103316	-0.000017
	88.2572	110.3716	189.1791	O	-0.575083	-0.684959	0.000023
	233.4367	352.9049	528.6926	C	0.438317	0.067797	0.000018
	608.8274	826.7270	940.8484	C	1.820044	-0.494826	-0.000005
	1001.9162	1020.7731	1170.9137	O	0.368580	1.322686	0.000006
	1210.7400	1280.1206	1399.4517	H	-2.053635	0.489671	-0.902691
	1427.2349	1454.2020	1475.2436	H	-2.053427	0.490352	0.902240
	1479.0304	1499.4012	1617.4133	H	-2.589612	-0.963320	0.000385
	3047.6393	3087.4797	3139.2600	H	2.576366	0.286590	0.000853
	3171.7428	3193.1602	3233.4881	H	1.909670	-1.110765	-0.897258
			H	1.909107	-1.112277	0.896257	
2b				C	1.803082	0.023083	-0.005105
	49.8617	146.0928	221.4032	O	0.616636	-0.751659	0.010023
	329.1654	485.9250	584.2199	C	-0.599415	-0.167399	-0.000125
	590.2017	810.0946	1009.6333	C	-0.655968	1.340151	0.001290
	1067.7498	1133.8802	1183.4882	O	-1.571826	-0.863405	-0.004952
	1200.2872	1298.7857	1407.2398	H	1.863199	0.692142	0.854313
	1472.1619	1485.0626	1496.4193	H	1.893827	0.601598	-0.925742
	1504.6862	1520.2206	1870.3551	H	2.621327	-0.689281	0.044275
	3049.1286	3074.7957	3120.7244	H	-1.698651	1.636698	-0.029966
	3143.7639	3168.6956	3189.5677	H	-0.133270	1.757275	-0.859220
			H	-0.191114	1.747073	0.899413	
2b⁺				C	-1.865197	0.115971	0.000000
	75.1273	183.4823	200.9268	O	-0.646508	-0.702722	0.000000
	269.6716	390.8456	529.8808	C	0.500294	-0.177867	0.000000
	574.3197	793.7364	955.1417	C	0.831458	1.278922	0.000000
	1018.3433	1025.2366	1172.8726	O	1.515408	-0.923259	0.000000
	1183.4692	1313.8283	1399.2286	H	-1.886628	0.719358	-0.902805
	1439.9480	1460.6382	1478.4954	H	-1.886628	0.719358	0.902805
	1494.9936	1505.3992	1649.0201	H	-2.666488	-0.612348	0.000000
	3047.1793	3092.6985	3136.8674	H	1.907083	1.440149	0.000000
	3167.2205	3202.1545	3227.4819	H	0.391071	1.719587	0.896981
			H	0.391071	1.719587	-0.896982	
3a	69.1359	169.3452	195.2418	O	2.230064	-0.094728	-0.097205
	265.4509	394.4626	671.5594	C	0.869593	-0.460149	0.012061
	696.3177	885.6646	911.8908	C	-0.050375	0.750511	-0.016508
	1066.8267	1090.8967	1115.2822	C	-1.512671	0.409349	-0.003805
	1198.8613	1307.0138	1332.5754	O	-1.950640	-0.708472	0.016000
	1400.0761	1419.4270	1429.7300	H	2.500536	0.332452	0.715444

	1455.8101	1507.8797	1846.8219	H	0.681647	-1.051631	0.912491
	2906.7044	3037.7362	3048.6470	H	0.654127	-1.103530	-0.838949
	3076.4800	3131.1557	3903.6093	H	0.147530	1.354883	-0.907302
				H	0.140829	1.415393	0.833679
				H	-2.199348	1.279776	-0.016213
				O	2.099424	-0.088082	-0.223341
	58.6881	168.0469	197.1825	C	0.841704	-0.433692	0.194557
	343.9818	388.2061	616.7882	C	-0.029447	0.834049	-0.000927
	716.4249	796.7869	853.1887	C	-1.484925	0.376448	0.041933
3a⁺	944.3064	1048.0166	1109.9059	O	-1.844260	-0.740423	-0.096365
	1145.4510	1165.2397	1220.8938	H	2.750493	-0.126243	0.487253
	1250.7024	1319.7252	1377.8238	H	0.799765	-0.793078	1.221576
	1438.2230	1486.9940	1816.8818	H	0.411109	-1.195198	-0.481799
	2876.2797	2909.2011	3055.6709	H	0.094773	1.264287	-1.001376
	3127.0200	3144.3591	3813.6356	H	0.158779	1.620470	0.729525
				H	-2.220225	1.196974	0.189086
	118.6755	167.0018	252.6354	O	-1.473770	-0.774794	-0.348909
	405.1319	509.5012	638.0279	C	-1.123471	0.363748	0.399124
	781.2550	855.1836	968.8091	H	-0.762385	-1.409492	-0.232521
	976.0824	1101.0780	1129.0956	H	-0.953163	0.111317	1.451655
3b	1229.3515	1261.1491	1392.6073	H	-1.975506	1.041642	0.358816
	1407.5722	1429.1483	1430.5703	C	0.108117	1.065731	-0.155777
	1450.3713	1522.8620	1838.6246	C	1.347517	0.219464	-0.115939
	2924.2348	3026.7682	3047.0124	O	1.367669	-0.938919	0.210912
	3086.1803	3113.1877	3856.1846	H	0.314848	1.995946	0.382781
				H	-0.052296	1.351743	-1.200691
				H	2.284331	0.724889	-0.420507
	202.3424	236.2652	282.9530	O	-1.086415	-0.850869	-0.299345
	432.6065	489.4112	622.0639	C	-1.139871	0.429772	0.274930
	823.2014	874.0702	910.4074	H	-1.419833	-1.532949	0.297544
	934.9053	1033.9475	1094.3661	H	-1.235617	0.386382	1.358972
3b⁺	1177.0993	1211.3810	1246.7789	H	-2.001143	0.962320	-0.145173
	1280.9404	1322.5030	1411.2164	C	0.125385	1.156485	-0.155539
	1436.2497	1480.7505	1727.3114	C	1.277304	0.206905	0.026730
	2991.3282	3026.7166	3049.4743	O	1.130499	-0.981914	0.097378
	3128.9817	3144.9763	3806.2497	H	0.295636	2.087747	0.382746
				H	0.127882	1.391911	-1.226667
				H	2.303494	0.607883	0.071593
	51.3197	108.4122	258.4542	O	-2.318906	-0.079441	0.008134
	297.5555	409.3541	534.3087	C	-1.031817	0.470163	0.168507
	791.6465	880.6215	982.9770	C	0.072040	-0.488164	-0.285793
	1086.5876	1094.5673	1126.6553	H	-2.413306	-0.818936	0.608961
3c	1202.1773	1275.3035	1327.3808	H	-0.853571	0.772573	1.205730
	1406.6444	1434.0684	1440.2754	H	-1.014958	1.374225	-0.441865
	1467.6000	1515.9315	1855.8562	H	-0.170384	-0.823223	-1.297776
	2894.1817	3029.6848	3061.4502	H	0.132804	-1.354714	0.373021
	3093.8072	3129.1624	3900.1258	C	1.408876	0.197549	-0.317135
				O	2.335230	-0.076472	0.393894
				H	1.494224	1.020088	-1.057764
				O	2.231172	-0.192011	0.071859

	364.8197	384.7461	451.1540	C	1.080825	0.519171	-0.191637
	725.5454	833.0987	843.2946	C	-0.058825	-0.458551	0.241824
	926.8765	1048.8268	1099.2554	H	2.590996	-0.603817	-0.721431
	1159.3631	1208.1622	1234.7825	H	0.974017	0.815069	-1.234480
	1252.7785	1372.5788	1387.6553	H	1.053566	1.396119	0.459651
	1449.5912	1508.8735	1819.3825	H	0.069905	-0.755656	1.287688
	2947.7813	3051.9982	3064.1490	H	-0.126234	-1.339200	-0.391585
	3133.2616	3176.3637	3827.4534	C	-1.399239	0.314204	0.216255
				O	-2.339638	-0.192263	-0.283048
				H	-1.431093	1.312723	0.691012
4a	73.1820	192.3983	199.9454	C	2.139134	-0.153757	0.000099
	225.9139	379.6684	740.5766	O	0.764340	-0.436900	-0.000294
	740.7899	885.2256	1071.9594	C	-0.018354	0.704660	0.000062
	1117.9250	1189.6411	1197.5402	C	-1.487963	0.377762	-0.000070
	1266.2870	1269.0145	1411.0242	O	-1.956898	-0.721179	0.000126
	1417.4533	1460.6093	1495.4526	H	2.432394	0.415493	0.890562
	1501.1341	1513.0545	1875.3866	H	2.432770	0.416215	-0.889776
	2890.6938	2948.5780	2969.8026	H	2.664286	-1.105635	-0.000176
	2991.8437	3043.1358	3153.4251	H	0.172568	1.341718	-0.880232
				H	0.172480	1.341196	0.880773
			H	-2.130940	1.283657	-0.000359	
4a ⁺	140.0509	150.9182	198.6729	C	1.551395	-0.696351	0.168239
	321.6099	419.9067	528.5268	O	0.997558	0.463785	-0.432852
	585.4359	794.4346	929.4614	C	-0.017436	1.067843	0.174136
	1018.3422	1073.4145	1146.6190	C	-1.414632	0.168566	0.023983
	1183.1428	1254.7707	1293.6732	O	-1.401115	-0.991622	-0.082719
	1329.9494	1437.7435	1450.3564	H	0.848038	-1.524143	-0.018040
	1476.4894	1507.3591	1938.9873	H	1.681667	-0.557842	1.241536
	2954.6264	2974.1263	3008.2483	H	2.489271	-0.895953	-0.338714
	3107.9171	3160.9494	3200.7860	H	-0.243685	2.018734	-0.304098
				H	0.042671	1.123076	1.269924
			H	-2.305470	0.818471	0.075805	
4b	72.8997	97.0171	218.5364	C	-2.257104	-0.116179	0.000001
	224.1303	436.6979	533.8941	O	-0.996986	0.502197	-0.000001
	748.9404	1020.2769	1063.6042	C	0.058161	-0.412299	-0.000001
	1121.0318	1192.0707	1195.3313	H	-2.395393	-0.741779	0.889620
	1251.1494	1260.2454	1368.0402	H	-2.395394	-0.741782	-0.889617
	1420.0753	1475.6902	1496.2055	H	-3.006971	0.671201	0.000000
	1498.0770	1517.7063	1862.1869	H	0.037408	-1.064230	-0.884458
	2932.5434	2982.3739	2996.1370	H	0.037408	-1.064230	0.884457
	3017.2028	3049.1603	3147.1058	C	1.361651	0.350321	0.000000
				O	2.434362	-0.182459	0.000000
			H	1.247688	1.451853	0.000001	
4b ⁺	140.0407	150.9074	198.6319	C	-1.551400	0.696351	-0.168232
	321.6099	419.9047	528.5118	O	-0.997554	-0.463785	0.432856
	585.4278	794.4392	929.4557	C	0.017431	-1.067841	-0.174147
	1018.3402	1073.4111	1146.6159	H	-1.681764	0.557799	-1.241513
	1183.1376	1254.7683	1293.6730	H	-0.847999	1.524126	0.017952
	1329.9469	1437.7443	1450.3458	H	-2.489230	0.896001	0.338785
	1476.4891	1507.3602	1938.9900	H	-0.042678	-1.123053	-1.269935

	2954.6253	2974.1294	3008.2524	H	0.243679	-2.018742	0.304070
	3107.9150	3160.9507	3200.7909	C	1.414638	-0.168567	-0.023974
				O	1.401117	0.991622	0.082709
				H	2.305476	-0.818475	-0.075758
	139.8263	181.8839	208.7365	C	-1.610794	-0.619923	0.259395
	275.7590	409.2846	715.0985	O	-0.985246	0.364378	-0.534378
	781.1193	844.3143	1006.8608	C	0.082888	0.992796	0.084364
	1112.4478	1194.5975	1206.6082	C	1.356904	0.183164	0.180087
	1257.9213	1325.7732	1396.9984	O	1.489802	-0.948708	-0.186523
4c	1413.7874	1452.7267	1491.7178	H	-2.000509	-0.182749	1.186771
	1510.8111	1520.8226	1864.7329	H	-0.929356	-1.437211	0.502814
	2875.9706	2960.7834	3006.8149	H	-2.442745	-1.011392	-0.320683
	3066.0016	3095.2346	3157.3026	H	-0.161097	1.331667	1.105576
				H	0.321695	1.895101	-0.487630
				H	2.201589	0.743002	0.637286
				C	-1.551401	-0.696351	0.168232
	140.0410	150.9076	198.6337	O	-0.997554	0.463785	-0.432856
	321.6098	419.9047	528.5104	C	0.017431	1.067841	0.174147
	585.4273	794.4392	929.4554	C	1.414638	0.168567	0.023974
4c⁺	1018.3400	1073.4115	1146.6161	O	1.401118	-0.991622	-0.082708
	1183.1376	1254.7680	1293.6731	H	-1.681765	-0.557799	1.241513
	1329.9470	1437.7446	1450.3466	H	-0.848001	-1.524127	-0.017952
	1476.4892	1507.3603	1938.9906	H	-2.489231	-0.896000	-0.338785
	2954.6262	2974.1295	3008.2527	H	-0.042678	1.123052	1.269936
	3107.9151	3160.9506	3200.7908	H	0.243679	2.018742	-0.304070
				H	2.305476	0.818476	0.075757
				C	0.786869	-0.636227	0.023685
	143.8182	180.6507	227.3979	C	-0.426720	-0.100579	0.016777
	267.8834	326.6453	429.9584	C	-0.719227	1.360918	0.005531
	461.6546	602.2858	835.8788	O	-1.503660	-0.951641	-0.054084
	847.9006	1022.2487	1067.2558	O	1.914659	0.143537	-0.073406
5a	1153.9428	1215.7779	1267.8192	H	0.918178	-1.711599	0.025521
	1334.4367	1395.9248	1442.3518	H	-1.215898	1.647494	-0.923969
	1486.6675	1494.8503	1829.3201	H	0.198189	1.934946	0.102458
	3036.2911	3094.5663	3169.1391	H	-1.382970	1.627770	0.833704
	3192.5049	3905.5716	3924.3180	H	-2.273572	-0.501805	0.293618
				H	2.622544	-0.276650	0.412633
				C	-0.843999	-0.614987	0.000000
	62.6447	236.5430	275.0202	C	0.459337	-0.093262	0.000000
	454.8116	462.9097	590.2355	C	0.790667	1.345393	0.000000
	602.9597	621.8014	844.6352	O	1.385255	-1.009353	0.000000
	904.7267	1034.5995	1037.2931	O	-1.845789	0.211030	0.000000
5a⁺	1163.5127	1245.3273	1347.7542	H	-1.005362	-1.687403	0.000000
	1405.0949	1438.4250	1474.3604	H	1.389200	1.582035	0.883235
	1494.6164	1506.4500	1707.2744	H	-0.101217	1.963462	0.000003
	3048.6179	3113.6800	3188.8438	H	1.389195	1.582036	-0.883238
	3199.4991	3797.9464	3811.6156	H	2.279047	-0.642313	0.000000
				H	-2.702622	-0.234091	0.000000
				C	-0.766422	-0.628937	-0.000631

	250.4499	294.4122	404.7745	C	0.402164	0.002236	-0.001691
	570.6562	613.1712	773.3806	C	1.714012	-0.707937	0.000856
	892.1996	1022.5178	1072.0251	O	0.436054	1.369596	-0.001371
	1171.4978	1217.8243	1260.8758	O	-1.955943	0.045180	0.007818
	1366.4931	1409.4060	1436.6023	H	-0.797643	-1.709867	0.001408
	1475.0052	1500.6099	1843.5779	H	2.304095	-0.439324	-0.880166
	3024.3968	3075.5382	3148.6917	H	1.577418	-1.787257	-0.002433
	3212.6553	3924.8840	3946.0157	H	2.298361	-0.444405	0.887224
				H	1.348024	1.657407	-0.004234
				H	-2.669665	-0.586936	-0.044572
				C	-0.791719	-0.657066	0.000000
				C	0.436223	0.029781	0.000000
				C	1.737480	-0.670860	0.000000
				O	0.359060	1.325245	0.000000
				O	-1.891903	0.026336	0.000000
5b⁺				H	-0.812542	-1.739949	0.000000
				H	2.312622	-0.380726	-0.882915
				H	1.616985	-1.750300	-0.000001
				H	2.312621	-0.380727	0.882916
				H	1.224338	1.755177	0.000000
				H	-2.683188	-0.527252	0.000000
				O	-1.827862	-0.079110	-0.390591
				C	-0.855047	0.368466	0.528999
				C	0.546836	0.037964	0.104533
				C	1.459835	0.958464	-0.191664
				O	0.752353	-1.299912	0.052455
6a				H	-1.631617	0.310923	-1.243322
				H	-1.072473	-0.142313	1.467456
				H	-0.927195	1.446025	0.702145
				H	2.467542	0.695107	-0.487785
				H	1.215361	2.007142	-0.126564
				H	1.642715	-1.474077	-0.258053
				O	1.810552	0.165359	-0.000127
				C	0.760578	-0.716649	-0.000006
				C	-0.529577	0.011537	0.000042
				C	-1.752285	-0.690086	-0.000023
				O	-0.461735	1.291308	0.000074
				H	2.647317	-0.304322	0.000455
6a⁺				H	0.731686	-1.387831	0.877383
				H	0.731562	-1.387659	-0.877512
				H	-2.701680	-0.169993	-0.000786
				H	-1.750629	-1.771102	0.000609
				H	-1.321087	1.738757	0.000191
				O	1.911331	0.087144	-0.008553
				C	0.760297	-0.710475	-0.083557
				C	-0.531122	0.058999	-0.021618
				C	-0.632036	1.381683	-0.041594

	1128.5875	1194.6617	1228.7025	O	-1.574886	-0.805515	0.064033
	1353.7263	1398.3076	1436.8108	H	1.916893	0.525522	0.843434
	1462.7407	1511.5856	1747.7709	H	0.734501	-1.473489	0.703193
	3024.0963	3101.9883	3176.6993	H	0.806334	-1.240562	-1.036149
	3280.9698	3888.9680	3890.7619	H	-1.589992	1.880884	0.020545
				H	0.254608	1.985369	-0.150469
				H	-2.396743	-0.311991	0.056216
				O	-1.791463	0.223629	0.000023
	90.3883	222.1437	293.2617	C	-0.777800	-0.723244	-0.000001
	353.8600	474.9293	501.7447	C	0.530312	-0.015786	-0.000003
	535.3016	657.9967	838.8289	C	0.634205	1.392388	-0.000005
	893.9896	992.7164	1007.9638	O	1.560933	-0.785520	0.000002
6b ⁺	1153.8361	1190.3632	1235.9273	H	-2.650214	-0.202405	-0.000113
	1262.7409	1418.5356	1442.1187	H	-0.782147	-1.380777	-0.881590
	1471.4192	1542.1685	1579.9951	H	-0.782136	-1.380804	0.881568
	2986.9843	3020.1197	3164.0211	H	1.600187	1.882301	-0.000001
	3291.3452	3762.7833	3903.9067	H	-0.273242	1.978836	-0.000009
				H	2.411492	-0.322173	0.000000
				C	-1.809941	-0.078727	0.164978
	60.4569	164.9025	313.1222	O	-0.605615	-0.694121	-0.270248
	353.8027	460.8909	597.5912	C	0.542888	-0.042894	-0.051542
	683.3247	689.3536	762.7790	C	1.695356	-0.684974	0.122648
	882.3683	968.0916	1139.2577	O	0.386780	1.301956	-0.071417
7a	1184.5805	1190.2841	1241.1128	H	-2.016212	0.835882	-0.388606
	1392.2744	1445.7690	1493.6536	H	-1.770055	0.145487	1.232646
	1511.4721	1517.8162	1750.7594	H	-2.593290	-0.807209	-0.023204
	3051.5714	3130.5640	3168.5730	H	2.626698	-0.145277	0.198964
	3198.3411	3298.6812	3911.3731	H	1.706525	-1.761167	0.155627
				H	1.227189	1.709175	0.141386
				C	-1.873737	-0.095055	0.000005
	128.2496	193.3851	277.8373	O	-0.548835	-0.712274	-0.000005
	362.2752	429.6274	563.6709	C	0.504696	-0.000723	-0.000002
	627.9115	678.2364	833.9955	C	1.757441	-0.670043	0.000003
	869.6061	1000.7210	1068.3834	O	0.366030	1.287248	-0.000002
7a ⁺	1171.7281	1175.8053	1236.2728	H	-1.980225	0.509220	-0.896764
	1457.8979	1460.4379	1477.7032	H	-1.980107	0.509477	0.896614
	1495.2918	1549.9620	1653.8264	H	-2.559482	-0.932303	0.000162
	3090.2840	3182.5614	3192.6856	H	2.682962	-0.112926	0.000004
	3231.2139	3308.3108	3814.6472	H	1.767383	-1.749327	0.000005
				H	1.201500	1.771000	0.000003
				C	1.845017	-0.029622	0.000005
	130.8340	219.8431	342.5042	O	0.609716	-0.709914	-0.000005
	349.3954	502.2975	576.4462	H	1.948760	0.592733	0.891708
	669.0707	691.2296	737.8298	H	1.948386	0.593293	-0.891353
	913.7090	992.4845	1140.9392	H	2.612474	-0.797634	-0.000451
7b	1189.0510	1232.1175	1247.0948	C	-0.497789	0.033825	0.000030

	1501.1763	1521.8420	1727.2126	C	-0.582174	1.367502	-0.000056
	3037.0166	3104.0485	3173.6287	O	-1.545928	-0.810931	0.000017
	3204.4777	3296.8309	3917.3321	H	-1.549114	1.846415	0.000048
				H	0.291066	1.995700	0.000176
				H	-2.352197	-0.293975	-0.000104
				C	1.895672	-0.017827	-0.000020
	161.8218	170.2566	301.3365	O	0.595234	-0.670789	-0.000087
	312.1209	483.5010	544.6361	H	2.000589	0.578101	0.902934
	569.2381	650.4236	823.0167	H	2.000575	0.578314	-0.902835
	869.6860	1012.4465	1076.6247	H	2.605810	-0.835166	-0.000122
7b ⁺	1176.5890	1197.2247	1238.3917	C	-0.503598	-0.032669	0.000001
	1451.7482	1474.0295	1498.5841	C	-0.622933	1.389875	0.000172
	1511.9919	1552.2176	1655.8664	O	-1.532164	-0.814033	-0.000082
	3085.4687	3185.3558	3189.2281	H	-1.600878	1.849416	0.000240
	3222.4017	3305.5043	3824.8116	H	0.252051	2.020479	0.000235
				H	-2.377548	-0.348851	-0.000018
				O	2.120370	-0.210038	-0.379408
	64.6582	237.6108	244.3931	C	1.014105	-0.223865	0.510903
	300.5175	351.5775	554.3538	C	-0.018710	0.792878	0.141324
	669.5933	780.6919	939.7753	C	-1.292170	0.528943	-0.118421
	976.6085	1033.6934	1076.3135	O	-1.818044	-0.723399	-0.038475
8a	1137.0712	1214.2796	1279.0394	H	1.778399	-0.335290	-1.265173
	1306.9926	1377.0872	1415.6436	H	1.434428	0.001752	1.491870
	1464.8527	1519.0809	1775.9709	H	0.563341	-1.218037	0.566851
	3053.3193	3101.7066	3177.1025	H	0.304794	1.821691	0.055878
	3214.8937	3896.6861	3942.7437	H	-1.984750	1.314501	-0.400362
				H	-2.734166	-0.704859	-0.308833
				O	2.239607	0.056599	-0.000067
	87.8981	198.4431	287.7799	C	0.945912	-0.418442	0.000046
	318.2963	401.7578	576.1844	C	0.005850	0.698910	0.000023
	645.9103	686.6192	924.1631	C	-1.381511	0.548422	0.000003
	995.3877	1018.0033	1140.2462	O	-1.890679	-0.638114	-0.000025
8a ⁺	1183.9055	1227.4894	1231.5608	H	2.867567	-0.668447	0.000078
	1277.8782	1353.4716	1378.4272	H	0.709110	-1.062302	0.870586
	1408.8966	1534.3609	1654.3537	H	0.709015	-1.062459	-0.870349
	2901.8621	2904.5694	3187.6537	H	0.400528	1.708270	0.000021
	3210.6474	3782.0523	3894.2415	H	-2.041070	1.410494	0.000010
				H	-2.858082	-0.646773	-0.000042
				C	0.064225	-0.198441	0.442904
	98.7854	200.6151	205.7684	C	1.136445	0.303815	-0.150163
	300.5409	330.0333	456.8743	O	2.359811	-0.276238	-0.065085
	579.0849	858.5369	962.8745	C	-1.283263	0.438744	0.334809
	966.9740	1036.1007	1108.0939	O	-2.186204	-0.275873	-0.497681
8b	1184.2016	1206.6897	1264.0211	H	0.160046	-1.116270	1.013304
	1358.0496	1379.3347	1385.8284	H	1.079522	1.219425	-0.732063
	1428.4124	1528.2686	1784.4047	H	2.993191	0.233763	-0.567208

	3178.3046	3901.3130	3933.3531	H	-1.193876	1.429412	-0.112043
				H	-1.718438	0.570500	1.332336
				H	-2.213738	-1.184654	-0.197496
				C	-0.005506	0.585126	0.272423
	68.3266	153.0461	291.3394	C	1.038934	-0.099973	-0.343469
	356.3396	407.0350	553.3973	O	2.199317	-0.104258	0.215515
	642.4269	864.4920	939.3832	C	-1.377861	0.529150	-0.302900
	999.2784	1032.7281	1080.6450	O	-1.738697	-0.772288	0.142857
8b⁺	1176.4599	1191.5819	1334.9815	H	0.171189	1.021730	1.248711
	1362.7272	1367.4024	1391.1035	H	0.898333	-0.622701	-1.286102
	1403.7749	1524.1482	1657.7419	H	2.873672	-0.580457	-0.289368
	3112.2048	3175.6538	3176.5481	H	-1.396369	0.527371	-1.389671
	3203.6335	3781.7175	3838.4633	H	-2.030091	1.312688	0.073396
				H	-2.135090	-0.732088	1.019739
				C	0.092691	0.741371	0.000254
	120.6660	198.5723	217.0376	C	0.947079	-0.267684	-0.000052
	256.3596	304.1060	424.6977	O	2.294990	-0.071354	-0.000352
	659.2196	817.8103	939.4492	H	0.466241	1.758090	0.000629
	959.2825	1058.7264	1136.1233	H	0.602583	-1.294595	-0.000428
8c	1178.2541	1197.9462	1255.7937	H	2.735141	-0.919214	0.002154
	1279.0773	1345.9956	1375.1882	C	-1.390235	0.567355	-0.000107
	1474.7746	1532.7600	1795.6396	O	-1.720133	-0.807622	0.000040
	2987.8410	3008.4112	3196.1734	H	-1.813734	1.065536	-0.882273
	3197.9619	3929.9157	3937.9806	H	-1.814131	1.065752	0.881736
				H	-2.672164	-0.890011	0.000104
				C	-0.068722	0.756061	0.000000
	174.7030	203.9833	216.5708	C	-0.968312	-0.312651	0.000000
	293.2733	433.7589	640.8905	O	-2.229864	-0.051217	0.000000
	654.5660	741.2238	930.3489	H	-0.458565	1.767161	0.000000
	943.3505	1017.2778	1156.8861	H	-0.619762	-1.340748	0.000000
	1202.7036	1228.7662	1230.3402	H	-2.788285	-0.842082	0.000000
8c⁺	1333.8118	1377.2159	1378.0832	C	1.376600	0.550686	0.000000
	1399.5251	1482.1213	1672.1978	O	1.684512	-0.800102	0.000000
	2929.5477	2941.6854	3198.3115	H	1.779132	1.097548	0.872763
	3209.9440	3775.3071	3902.4504	H	1.779132	1.097548	-0.872762
				H	2.633763	-0.933450	0.000000
				C	-2.171098	-0.162403	0.156993
	50.0062	175.8441	189.8915	O	-0.845968	-0.386732	-0.260644
	214.1431	376.4038	556.6746	C	-0.015263	0.670651	-0.082876
	732.1704	743.7586	873.0733	C	1.298515	0.538796	0.043894
	1001.2402	1117.8894	1177.8169	O	1.920051	-0.672804	0.050845
	1187.9572	1238.8081	1286.9462	H	-2.607141	0.706356	-0.348312
9a	1338.4199	1436.0783	1497.2379	H	-2.229124	-0.007691	1.238564
	1499.6333	1520.2127	1810.4127	H	-2.742557	-1.048659	-0.107580
	3011.2833	3070.3305	3148.1341	H	-0.459906	1.659653	-0.087873
	3179.2381	3213.1960	3944.5756	H	1.912119	1.426081	0.126883
				H	2.861023	-0.541712	0.148651

			C	-2.227389	-0.179008	0.000046	
	65.2727	162.1638	202.3358	O	-0.785311	-0.332575	-0.000086
	368.7642	397.6631	604.2091	C	-0.021602	0.692132	-0.000016
	723.5442	857.9728	957.1083	C	1.366174	0.519246	0.000012
	973.1150	1103.3521	1175.4129	O	1.856802	-0.678965	0.000015
9a⁺	1190.0437	1262.0083	1322.4065	H	-2.496881	0.874623	-0.000892
	1408.7952	1465.2460	1472.6056	H	-2.588494	-0.680710	0.892612
	1504.6209	1576.5713	1706.7606	H	-2.588769	-0.682326	-0.891492
	3081.4958	3179.8175	3192.8684	H	-0.439903	1.694012	0.000010
	3200.1762	3209.3347	3808.5580	H	2.016686	1.385877	0.000032
				H	2.822335	-0.693368	0.000040
				C	-1.423719	-0.848368	0.058886
	67.4699	166.4594	232.5707	O	-1.245060	0.548306	-0.085688
	288.5221	360.5425	543.3503	C	0.001181	1.055534	0.016866
	754.4810	817.4407	912.6913	C	1.195272	0.469668	0.038817
	929.1195	1059.3113	1186.2776	O	1.431228	-0.875880	-0.093145
9b	1200.1250	1239.1480	1282.9224	H	-1.031109	-1.195787	1.016231
	1377.6573	1439.0930	1498.0464	H	-0.936502	-1.400761	-0.744207
	1503.7580	1520.6406	1794.3464	H	-2.497173	-1.017409	0.022888
	3044.4461	3120.0321	3152.1352	H	-0.021723	2.134881	0.067154
	3189.7580	3224.6146	3934.4915	H	2.063093	1.111120	0.122829
				H	2.297667	-1.072451	0.258360
				C	-1.485951	-0.824430	0.000000
	143.9061	157.4608	237.5777	O	-1.155968	0.592310	0.000000
	354.0160	431.6083	596.4565	C	0.027188	1.071695	0.000000
	814.4140	845.7470	861.2983	C	1.257944	0.402752	0.000000
	959.2039	1058.7612	1168.5557	O	1.340028	-0.895403	0.000000
9b⁺	1204.0945	1270.8714	1330.4869	H	-1.083251	-1.285191	0.897602
	1431.8143	1468.2154	1475.9352	H	-1.083254	-1.285190	-0.897604
	1500.9379	1572.5838	1702.0557	H	-2.568409	-0.848417	0.000002
	3089.9462	3193.2349	3197.0161	H	0.053922	2.155413	0.000000
	3212.3013	3224.2530	3801.3968	H	2.161348	1.001835	0.000000
				H	2.252073	-1.213804	0.000000
				C	0.027006	0.236792	-0.210932
	86.1553	169.0090	212.6304	C	1.168054	-0.365514	0.085541
	219.6140	359.9220	471.4661	O	2.357785	0.303191	0.021412
	553.4236	856.0451	932.7003	O	-1.135632	-0.469309	-0.295471
	1041.8701	1149.4549	1194.6210	C	-2.248268	0.211090	0.238772
9c	1200.4469	1226.1220	1281.5921	H	-0.018020	1.295499	-0.452298
	1329.0999	1372.8676	1489.2020	H	1.192255	-1.421502	0.329006
	1498.4577	1525.8524	1800.2841	H	3.015733	-0.183397	0.514468
	3009.7838	3068.8273	3151.4031	H	-3.122294	-0.409463	0.056135
	3153.6993	3185.2009	3937.3289	H	-2.390847	1.181030	-0.250080
				H	-2.134804	0.372573	1.314957
				C	0.016255	0.263763	-0.000016

	269.4268	481.4148	525.8216	C	1.244766	-0.395244	0.000015
	580.9191	917.1009	946.6657	O	2.318683	0.333520	0.000002
	966.2953	1151.6461	1174.8548	O	-1.049063	-0.448150	-0.000029
	1196.9368	1311.2369	1345.8320	C	-2.355754	0.182283	0.000021
	1372.1494	1444.2870	1472.9147	H	-0.037251	1.349580	-0.000053
	1504.3437	1534.7018	1717.4482	H	1.301182	-1.478618	0.000040
	3082.0299	3170.3148	3193.5363	H	3.131936	-0.186879	0.000019
	3197.0230	3199.7146	3811.4535	H	-2.865165	-0.167646	-0.892666
				H	-2.253511	1.264847	0.000934
				H	-2.865754	-0.169058	0.891818
				C	0.066766	0.701850	0.026399
	163.3422	203.9319	251.6385	C	0.907750	-0.326883	0.001720
	260.8815	367.3497	413.1497	O	2.260378	-0.091303	-0.078650
	645.9309	815.2189	937.5617	H	0.443565	1.715191	0.044431
	999.4135	1169.8382	1185.0474	H	0.591165	-1.362084	-0.026990
9d	1190.5504	1247.3297	1302.6965	H	2.718906	-0.717172	0.480954
	1334.3529	1364.3270	1489.2160	O	-1.283897	0.663888	0.004488
	1493.9941	1514.1261	1768.7035	C	-1.878493	-0.609393	-0.007152
	3008.5542	3066.6272	3159.4579	H	-2.953588	-0.452864	-0.019957
	3188.4032	3225.1520	3907.7703	H	-1.605259	-1.181514	0.885552
				H	-1.582782	-1.175675	-0.896491
				C	0.062502	0.724332	0.000000
	156.0063	203.3837	236.1437	C	0.943711	-0.362581	0.000000
	352.6513	405.6514	578.2037	O	2.211198	-0.074598	0.000000
	641.2670	891.9435	902.9284	H	0.460164	1.733858	0.000000
	948.1335	1152.6050	1173.0608	H	0.621168	-1.396962	0.000001
9d⁺	1207.7132	1316.0803	1357.5723	H	2.782748	-0.853070	0.000000
	1382.4285	1440.2260	1480.2294	O	-1.213860	0.655950	0.000000
	1509.9126	1534.1636	1712.7371	C	-1.925824	-0.607214	0.000000
	3074.6381	3172.8022	3198.3558	H	-2.974621	-0.337864	0.000000
	3207.6011	3219.0740	3809.6831	H	-1.675246	-1.162001	0.902037
				H	-1.675246	-1.162000	-0.902038

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