

Electronic supplementary information

Gas phase H^+ , H_3O^+ and NH_4^+ affinities of oxygen-bearing volatile organic compounds; DFT calculations for soft chemical ionisation mass spectrometry

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H₂O

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE
O -3.133500 0.572570 0.000000
H -2.163500 0.572570 0.000000
H -3.456830 -0.082380 0.638280

FINAL GEOMETRY OPTIMIZATION CYCLE
O -3.154794 0.628826 0.146509
H -2.205451 0.583985 -0.094060
H -3.466262 -0.150137 0.653801
H -3.738102 0.867536 -0.604500

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0: 0.00 cm⁻¹
1: 0.00 cm⁻¹
2: 0.00 cm⁻¹
3: 0.00 cm⁻¹
4: 0.00 cm⁻¹
5: 0.00 cm⁻¹
6: 1602.07 cm⁻¹
7: 3812.37 cm⁻¹
8: 3916.85 cm⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-76.65643341 Eh	
Total entropy correction	...	-0.02301514 Eh	-14.44 kcal/mol

Final Gibbs free energy	...	-76.67944855 Eh	

H₃O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	-3.143300	0.582520	-0.009690
H	-2.181760	0.555870	0.016270
H	-3.428770	-0.075630	0.631700
H	-3.810780	0.867450	-0.536530

FINAL GEOMETRY OPTIMIZATION CYCLE

O	-3.143249	0.582466	-0.009644
H	-2.181963	0.555810	0.016334
H	-3.428618	-0.075516	0.631590

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	765.88	cm** ⁻¹
7:	1672.08	cm** ⁻¹
8:	1673.09	cm** ⁻¹
9:	3579.20	cm** ⁻¹
10:	3673.93	cm** ⁻¹
11:	3674.28	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-76.65643341 Eh	
Total entropy correction	...	-0.02301514 Eh	-14.44 kcal/mol

Final Gibbs free energy	...	-76.67944855	

NH₃

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

N	-1.132050	0.684240	0.000000
H	-0.112050	0.684240	0.000000
H	-1.472050	0.891200	0.939130
H	-1.472050	-0.232550	-0.290330

FINAL GEOMETRY OPTIMIZATION CYCLE

N	-1.138118	0.696873	-0.011584
H	-0.123677	0.676480	0.007135
H	-1.463183	0.880309	0.932104
H	-1.463222	-0.226532	-0.278854

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
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3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	1006.15	cm** ⁻¹
7:	1667.64	cm** ⁻¹
8:	1667.71	cm** ⁻¹
9:	3476.45	cm** ⁻¹
10:	3602.45	cm** ⁻¹
11:	3602.87	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-56.50901226 Eh	
Total entropy correction	...	-0.02185055 Eh	-13.71 kcal/mol

Final Gibbs free energy	...	-56.53086281	

NH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

N	-1.138030	0.696680	-0.011400
H	-0.123580	0.676570	0.007040
H	-1.463280	0.880440	0.932140
H	-1.463310	-0.226560	-0.278980
H	-0.710250	0.157670	-0.396260

FINAL GEOMETRY OPTIMIZATION CYCLE

N	-1.125544	0.690092	-0.109914
H	-0.213311	1.164189	0.069980
H	-1.286626	0.600905	0.942534
H	-1.922125	0.037184	-0.263798
H	-0.350844	-0.307570	-0.386262

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	1488.64	cm** ⁻¹
7:	1488.79	cm** ⁻¹
8:	1488.94	cm** ⁻¹
9:	1726.32	cm** ⁻¹
10:	1726.41	cm** ⁻¹
11:	3368.50	cm** ⁻¹
12:	3471.05	cm** ⁻¹
13:	3471.10	cm** ⁻¹
14:	3471.16	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-56.83127180 Eh	
Total entropy correction	...	-0.02279770 Eh	-14.31 kcal/mol

Final Gibbs free energy	...	-56.85406951	

ACETONE C₃H₆O

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	1.302070	5.535510	0.395750
C	1.664750	4.137780	0.817770
H	2.062630	6.236460	0.750840
H	0.334710	5.808020	0.824240
H	1.261500	5.590780	-0.695110
C	0.803800	3.016300	0.302750
H	0.225390	2.595310	1.128540
H	1.440900	2.249180	-0.144780
H	0.114740	3.383300	-0.462600
O	2.604130	3.919790	1.582740

FINAL GEOMETRY OPTIMIZATION CYCLE

C	1.262204	5.541412	0.513412
C	1.766104	4.121529	0.688764
H	2.034985	6.250616	0.807348
H	0.367467	5.699283	1.124686
H	0.972136	5.717611	-0.527343
C	0.818387	3.013304	0.272473
H	-0.141266	3.116887	0.788936
H	1.256351	2.041341	0.496071
H	0.610856	3.083975	-0.800540
O	2.867395	3.886475	1.136334

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	20.63	cm** ⁻¹
7:	127.68	cm** ⁻¹
8:	382.04	cm** ⁻¹
9:	489.61	cm** ⁻¹
10:	535.56	cm** ⁻¹
11:	784.66	cm** ⁻¹
12:	882.98	cm** ⁻¹
13:	887.38	cm** ⁻¹
14:	1083.16	cm** ⁻¹
15:	1116.02	cm** ⁻¹
16:	1232.75	cm** ⁻¹
17:	1385.29	cm** ⁻¹
18:	1386.15	cm** ⁻¹
19:	1459.58	cm** ⁻¹
20:	1464.01	cm** ⁻¹
21:	1470.11	cm** ⁻¹
22:	1486.79	cm** ⁻¹
23:	1785.09	cm** ⁻¹
24:	3021.89	cm** ⁻¹
25:	3029.07	cm** ⁻¹
26:	3076.28	cm** ⁻¹
27:	3083.59	cm** ⁻¹
28:	3136.80	cm** ⁻¹
29:	3137.84	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-193.01976255 Eh	
Total entropy correction	...	-0.03450410 Eh	-21.65 kcal/mol

Final Gibbs free energy ... -193.05426665

PROTONATED ACETONE C₃H₇O⁺
CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	1.261780	5.541500	0.514800
C	1.766090	4.121620	0.688520
H	2.036930	6.250960	0.801700
H	0.372170	5.700210	1.133370
H	0.962970	5.716600	-0.523670
C	0.818630	3.013320	0.271530
H	-0.144900	3.121240	0.779680
H	1.253070	2.041560	0.502740
H	0.620160	3.078990	-0.803580
O	2.867730	3.886420	1.135050
H	3.910310	4.256720	1.574000

FINAL GEOMETRY OPTIMIZATION CYCLE

C	1.332383	5.519144	0.581991
C	1.732448	4.104210	0.674091
H	2.168282	6.214584	0.674610
H	0.618774	5.709296	1.398215
H	0.782822	5.698408	-0.346391
C	0.851481	3.002305	0.265626
H	-0.193640	3.235256	0.481038
H	1.157958	2.051865	0.700586
H	0.931154	2.923321	-0.831043
O	2.880373	3.761633	1.120737
H	3.462906	4.509118	1.354681

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	103.54	cm** ⁻¹
7:	134.94	cm** ⁻¹
8:	396.77	cm** ⁻¹
9:	482.49	cm** ⁻¹
10:	511.94	cm** ⁻¹
11:	718.22	cm** ⁻¹
12:	830.94	cm** ⁻¹
13:	922.95	cm** ⁻¹
14:	950.72	cm** ⁻¹
15:	1075.28	cm** ⁻¹
16:	1092.71	cm** ⁻¹
17:	1158.21	cm** ⁻¹
18:	1363.14	cm** ⁻¹
19:	1373.75	cm** ⁻¹
20:	1406.43	cm** ⁻¹
21:	1426.15	cm** ⁻¹
22:	1444.08	cm** ⁻¹
23:	1466.41	cm** ⁻¹
24:	1489.48	cm** ⁻¹
25:	1586.34	cm** ⁻¹
26:	2993.14	cm** ⁻¹
27:	3005.63	cm** ⁻¹
28:	3077.00	cm** ⁻¹
29:	3087.22	cm** ⁻¹
30:	3132.41	cm** ⁻¹
31:	3157.31	cm** ⁻¹
32:	3663.76	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-193.32788035 Eh	
Total entropy correction	...	-0.03402944 Eh	-21.35 kcal/mol

Final Gibbs free energy	...	-193.36190979	

PROPANOL C₃H₈O

CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-8.224000	0.622250	0.000000
C	-5.713600	2.996620	0.000000
H	-8.062390	-0.067670	-0.801750
H	-9.170600	1.104030	-0.129380
H	-8.216380	0.095140	0.931130
C	-3.529230	0.229250	0.000000
H	-5.668840	3.612760	0.873650
H	-5.656220	3.786460	-0.719550
O	-1.018830	2.800120	0.000000
H	-3.561740	-0.387660	-0.873650
H	-3.571450	-0.571880	0.708030
H	-1.184810	3.414100	-0.732380

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-6.651485	1.382288	-0.594038
C	-5.694778	1.769659	0.535828
H	-6.308008	1.785221	-1.548776
H	-7.658257	1.764563	-0.404508
H	-6.721226	0.293821	-0.693737
C	-4.274755	1.269611	0.318948
H	-6.053579	1.365833	1.489887
H	-5.663177	2.859308	0.645468
O	-3.752936	1.894661	-0.858331
H	-4.276953	0.175831	0.202298
H	-3.653591	1.517035	1.190609
H	-2.869344	1.555689	-1.027549

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	143.06	cm** ⁻¹
7:	223.17	cm** ⁻¹
8:	239.63	cm** ⁻¹
9:	325.28	cm** ⁻¹
10:	478.13	cm** ⁻¹
11:	774.84	cm** ⁻¹
12:	862.37	cm** ⁻¹
13:	926.07	cm** ⁻¹
14:	979.19	cm** ⁻¹
15:	1061.54	cm** ⁻¹
16:	1108.77	cm** ⁻¹
17:	1156.14	cm** ⁻¹
18:	1238.73	cm** ⁻¹
19:	1270.16	cm** ⁻¹
20:	1321.45	cm** ⁻¹
21:	1379.56	cm** ⁻¹
22:	1409.35	cm** ⁻¹
23:	1442.64	cm** ⁻¹
24:	1477.50	cm** ⁻¹
25:	1494.33	cm** ⁻¹
26:	1508.52	cm** ⁻¹
27:	1517.33	cm** ⁻¹
28:	2969.26	cm** ⁻¹
29:	2998.70	cm** ⁻¹
30:	3020.62	cm** ⁻¹
31:	3021.47	cm** ⁻¹

32: 3050.65 cm**⁻¹
33: 3080.15 cm**⁻¹
34: 3105.47 cm**⁻¹
35: 3845.34 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-194.19057708 Eh	
Total entropy correction	...	-0.03425568 Eh	-21.50 kcal/mol

Final Gibbs free energy	...	-194.22483276	

PROTONATED PROPANOL C₃H₉O⁺
CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-6.651440	1.382460	-0.594040
C	-5.694680	1.769850	0.535990
H	-6.308230	1.786600	-1.548370
H	-7.658680	1.763270	-0.404280
H	-6.719780	0.294000	-0.694840
C	-4.274750	1.269390	0.319090
H	-6.053640	1.366390	1.490150
H	-5.663360	2.859500	0.645360
O	-3.753340	1.893830	-0.858690
H	-4.277500	0.175670	0.203030
H	-3.653220	1.517140	1.190270
H	-2.869470	1.555420	-1.027570
H	-4.080580	1.239280	-1.778090

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-6.626012	1.351842	-0.622128
C	-5.695942	1.775574	0.521260
H	-6.336366	1.779769	-1.591697
H	-7.636199	1.718577	-0.436794
H	-6.680467	0.264620	-0.722660
C	-4.307016	1.207871	0.428074
H	-6.084016	1.400814	1.476399
H	-5.645329	2.863591	0.618538
O	-3.678129	1.748400	-0.903419
H	-4.265321	0.123336	0.331739
H	-3.608381	1.584257	1.171485
H	-2.804822	1.382609	-1.133154
H	-4.290669	1.671539	-1.659633

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	131.09	cm** ⁻¹
7:	196.95	cm** ⁻¹
8:	235.77	cm** ⁻¹
9:	313.43	cm** ⁻¹
10:	444.56	cm** ⁻¹
11:	635.11	cm** ⁻¹
12:	688.35	cm** ⁻¹
13:	768.51	cm** ⁻¹
14:	852.05	cm** ⁻¹
15:	921.45	cm** ⁻¹
16:	967.27	cm** ⁻¹
17:	1032.03	cm** ⁻¹
18:	1134.70	cm** ⁻¹
19:	1153.24	cm** ⁻¹
20:	1253.73	cm** ⁻¹
21:	1298.33	cm** ⁻¹
22:	1378.31	cm** ⁻¹
23:	1410.01	cm** ⁻¹
24:	1432.33	cm** ⁻¹
25:	1465.93	cm** ⁻¹
26:	1485.24	cm** ⁻¹
27:	1494.35	cm** ⁻¹
28:	1511.90	cm** ⁻¹
29:	1643.83	cm** ⁻¹

30: 2996.19 cm**⁻¹
31: 3035.98 cm**⁻¹
32: 3069.49 cm**⁻¹
33: 3086.29 cm**⁻¹
34: 3101.48 cm**⁻¹
35: 3123.21 cm**⁻¹
36: 3182.77 cm**⁻¹
37: 3638.85 cm**⁻¹
38: 3732.55 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-194.48710792 Eh	
Total entropy correction	...	-0.03497473 Eh	-21.95 kcal/mol

Final Gibbs free energy	...	-194.52208264	

2-BUTENAL C₄H₆O

CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.884730	1.584110	0.007920
C	-4.624080	0.816000	0.039200
C	-3.439970	1.439000	-0.036680
C	-2.138420	0.705760	-0.005320
H	-2.156130	-0.111910	0.722220
H	-1.333300	1.388840	0.283750
H	-1.902780	0.303120	-0.994920
H	-4.721570	-0.261090	0.113110
H	-3.384150	2.521740	-0.123640
O	-6.972130	1.023690	0.036870
H	-5.788740	2.681580	-0.042510

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.888147	1.575900	0.019316
C	-4.641512	0.813237	0.145493
C	-3.455968	1.382544	-0.109084
C	-2.126157	0.709675	-0.020795
H	-2.215718	-0.332768	0.290060
H	-1.476415	1.232214	0.690210
H	-1.614442	0.742627	-0.989323
H	-4.728892	-0.226260	0.449699
H	-3.447633	2.430405	-0.410461
O	-6.995990	1.126411	0.222502
H	-5.755126	2.636856	-0.287616

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
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3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	126.72	cm** ⁻¹
7:	197.70	cm** ⁻¹
8:	209.46	cm** ⁻¹
9:	295.01	cm** ⁻¹
10:	461.57	cm** ⁻¹
11:	544.56	cm** ⁻¹
12:	797.61	cm** ⁻¹
13:	942.42	cm** ⁻¹
14:	1002.19	cm** ⁻¹
15:	1026.63	cm** ⁻¹
16:	1070.17	cm** ⁻¹
17:	1093.13	cm** ⁻¹
18:	1166.00	cm** ⁻¹
19:	1279.96	cm** ⁻¹
20:	1328.00	cm** ⁻¹
21:	1409.31	cm** ⁻¹
22:	1416.00	cm** ⁻¹
23:	1476.30	cm** ⁻¹
24:	1482.85	cm** ⁻¹
25:	1696.63	cm** ⁻¹
26:	1760.22	cm** ⁻¹
27:	2867.66	cm** ⁻¹
28:	3015.14	cm** ⁻¹
29:	3058.45	cm** ⁻¹
30:	3099.84	cm** ⁻¹
31:	3117.48	cm** ⁻¹
32:	3157.47	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-231.08172136 Eh	
Total entropy correction	...	-0.03540424 Eh	-22.22 kcal/mol

Final Gibbs free energy	...	-231.11712560	

PROTONATED 2-BUTENAL C₄H₆O⁺
CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.888100	1.575870	0.019440
C	-4.641300	0.813400	0.145310
C	-3.455800	1.382770	-0.109220
C	-2.126190	0.709700	-0.020910
H	-2.216250	-0.332710	0.290000
H	-1.476710	1.231960	0.690560
H	-1.614200	0.742420	-0.989290
H	-4.728750	-0.226070	0.449580
H	-3.447360	2.430630	-0.410610
O	-6.995790	1.126070	0.222900
H	-5.755540	2.636800	-0.287760
H	-6.840770	0.091670	0.514260

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.797987	1.534428	0.024174
C	-4.632651	0.773098	0.155288
C	-3.427330	1.369141	-0.107688
C	-2.116531	0.713555	-0.022253
H	-2.167562	-0.330362	0.283317
H	-1.475682	1.276844	0.670797
H	-1.609765	0.795066	-0.994479
H	-4.691101	-0.268766	0.458126
H	-3.430929	2.416956	-0.407190
O	-7.002436	1.127763	0.228775
H	-5.761077	2.579277	-0.277196
H	-7.073709	0.195511	0.502587

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm ^{**} -1
1:	0.00	cm ^{**} -1
2:	0.00	cm ^{**} -1
3:	0.00	cm ^{**} -1
4:	0.00	cm ^{**} -1
5:	0.00	cm ^{**} -1
6:	128.27	cm ^{**} -1
7:	183.18	cm ^{**} -1
8:	210.41	cm ^{**} -1
9:	312.96	cm ^{**} -1
10:	465.45	cm ^{**} -1
11:	522.44	cm ^{**} -1
12:	702.32	cm ^{**} -1
13:	838.80	cm ^{**} -1
14:	934.39	cm ^{**} -1
15:	962.46	cm ^{**} -1
16:	1047.24	cm ^{**} -1
17:	1081.50	cm ^{**} -1
18:	1150.91	cm ^{**} -1
19:	1162.49	cm ^{**} -1
20:	1281.42	cm ^{**} -1
21:	1303.25	cm ^{**} -1
22:	1350.02	cm ^{**} -1
23:	1373.33	cm ^{**} -1
24:	1421.79	cm ^{**} -1
25:	1442.16	cm ^{**} -1
26:	1464.75	cm ^{**} -1
27:	1579.38	cm ^{**} -1
28:	1639.43	cm ^{**} -1
29:	3000.01	cm ^{**} -1
30:	3033.77	cm ^{**} -1
31:	3130.41	cm ^{**} -1

32: 3147.53 cm**⁻¹
33: 3161.44 cm**⁻¹
34: 3173.52 cm**⁻¹
35: 3688.84 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-231.39889650 Eh	
Total entropy correction	...	-0.03564902 Eh	-22.37 kcal/mol

Final Gibbs free energy	...	-231.43454552	

TRANS-2-HEPTANAL C₇H₁₂O
CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-4.539210	0.216170	0.012540
C	-3.193480	-0.390030	0.000100
C	-2.086170	0.366750	-0.016930
C	-0.714950	-0.250110	-0.041840
C	0.410100	0.788060	0.014770
H	-0.609420	-0.839950	-0.960660
H	-0.612820	-0.934320	0.809590
C	1.778080	0.104230	-0.038540
H	0.327860	1.378880	0.935740
H	0.315280	1.486980	-0.825840
C	2.918190	1.108410	-0.002070
H	1.857950	-0.492980	-0.954510
H	1.880930	-0.585870	0.807100
H	2.862030	1.798190	-0.850040
H	3.880070	0.587910	-0.051930
H	2.896950	1.694160	0.922170
H	-3.162260	-1.473980	-0.000440
H	-2.157820	1.452120	-0.021090
O	-5.547780	-0.477900	0.019070
H	-4.581890	1.317620	0.013750

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-4.415771	0.367508	0.253079
C	-3.093731	-0.262274	0.328974
C	-2.088585	0.142103	-0.459005
C	-0.697533	-0.402800	-0.453488
C	0.345950	0.661743	-0.065711
H	-0.458856	-0.776587	-1.458418
H	-0.631338	-1.256070	0.228874
C	1.780106	0.126170	-0.095231
H	0.114367	1.040289	0.936662
H	0.261088	1.518528	-0.745806
C	2.816761	1.182027	0.295745
H	2.002844	-0.254757	-1.099401
H	1.858020	-0.733075	0.581798
H	2.784850	2.038098	-0.385664
H	3.830576	0.773440	0.269541
H	2.635492	1.557514	1.307788
H	-2.972109	-1.064876	1.051358
H	-2.281716	0.957091	-1.158386
O	-5.367463	0.059276	0.939111
H	-4.501313	1.180993	-0.500879

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	43.74	cm** ⁻¹
7:	72.38	cm** ⁻¹
8:	105.57	cm** ⁻¹
9:	136.11	cm** ⁻¹
10:	159.19	cm** ⁻¹
11:	218.36	cm** ⁻¹
12:	243.25	cm** ⁻¹
13:	266.33	cm** ⁻¹
14:	323.34	cm** ⁻¹
15:	435.12	cm** ⁻¹

16: 502.92 cm**-1
 17: 569.89 cm**-1
 18: 738.80 cm**-1
 19: 795.21 cm**-1
 20: 836.59 cm**-1
 21: 904.39 cm**-1
 22: 939.14 cm**-1
 23: 1000.70 cm**-1
 24: 1007.43 cm**-1
 25: 1030.18 cm**-1
 26: 1046.41 cm**-1
 27: 1058.29 cm**-1
 28: 1110.27 cm**-1
 29: 1121.56 cm**-1
 30: 1175.83 cm**-1
 31: 1227.15 cm**-1
 32: 1265.73 cm**-1
 33: 1288.95 cm**-1
 34: 1318.87 cm**-1
 35: 1324.00 cm**-1
 36: 1336.02 cm**-1
 37: 1358.17 cm**-1
 38: 1392.96 cm**-1
 39: 1414.06 cm**-1
 40: 1417.32 cm**-1
 41: 1480.78 cm**-1
 42: 1488.14 cm**-1
 43: 1498.12 cm**-1
 44: 1499.46 cm**-1
 45: 1510.77 cm**-1
 46: 1691.74 cm**-1
 47: 1758.87 cm**-1
 48: 2867.53 cm**-1
 49: 2997.77 cm**-1
 50: 3002.20 cm**-1
 51: 3010.57 cm**-1
 52: 3018.56 cm**-1
 53: 3024.35 cm**-1
 54: 3043.03 cm**-1
 55: 3061.99 cm**-1
 56: 3079.61 cm**-1
 57: 3085.13 cm**-1
 58: 3104.01 cm**-1
 59: 3156.70 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-348.89053871 Eh	
Total entropy correction	...	-0.04525931 Eh	-28.40 kcal/mol

Final Gibbs free energy	...	-348.93579802	

PROTONATED TRANS-2-HEPTANAL C₇H₁₂O⁺
CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-4.414400	0.368230	0.255490
C	-3.092160	-0.261340	0.329720
C	-2.088650	0.141130	-0.461320
C	-0.697470	-0.403340	-0.456250
C	0.345570	0.661750	-0.068520
H	-0.458430	-0.777880	-1.460760
H	-0.630940	-1.256110	0.226750
C	1.779830	0.126430	-0.095940
H	0.112740	1.040830	0.933380
H	0.261160	1.518110	-0.749190
C	2.815630	1.181770	0.298490
H	2.004510	-0.253410	-1.100100
H	1.856340	-0.733680	0.580180
H	2.785480	2.038620	-0.382040
H	3.829520	0.773240	0.274360
H	2.631900	1.556230	1.310480
H	-2.969030	-1.062020	1.053980
H	-2.283680	0.954370	-1.162220
O	-5.364120	0.061990	0.945120
H	-4.502150	1.179430	-0.500690
H	-4.798430	-0.666120	0.040150

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-4.262599	0.369087	0.030411
C	-3.033132	-0.271151	0.169325
C	-2.005919	0.078842	-0.673106
C	-0.646342	-0.459170	-0.625149
C	0.332354	0.653226	-0.105618
H	-0.326318	-0.721721	-1.640730
H	-0.579679	-1.343652	0.011002
C	1.777847	0.140127	-0.079659
H	0.022935	0.959135	0.898400
H	0.257745	1.533530	-0.751846
C	2.745788	1.201944	0.447580
H	2.069407	-0.163822	-1.090712
H	1.832889	-0.756767	0.546607
H	2.738942	2.096599	-0.181284
H	3.766879	0.814029	0.461641
H	2.491754	1.502930	1.467932
H	-2.897630	-1.040447	0.924789
H	-2.198894	0.855401	-1.413462
O	-5.326046	0.143319	0.727000
H	-4.418439	1.142093	-0.718844
H	-5.218323	-0.545302	1.406793

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	38.51	cm** ⁻¹
7:	66.31	cm** ⁻¹
8:	104.77	cm** ⁻¹
9:	138.08	cm** ⁻¹
10:	163.94	cm** ⁻¹
11:	217.86	cm** ⁻¹
12:	240.13	cm** ⁻¹
13:	262.40	cm** ⁻¹

14: 338.85 cm**-1
15: 434.95 cm**-1
16: 496.61 cm**-1
17: 546.70 cm**-1
18: 705.53 cm**-1
19: 742.86 cm**-1
20: 808.88 cm**-1
21: 861.34 cm**-1
22: 910.77 cm**-1
23: 925.55 cm**-1
24: 950.82 cm**-1
25: 985.66 cm**-1
26: 1033.63 cm**-1
27: 1050.34 cm**-1
28: 1070.01 cm**-1
29: 1095.36 cm**-1
30: 1163.71 cm**-1
31: 1173.39 cm**-1
32: 1214.74 cm**-1
33: 1244.16 cm**-1
34: 1279.99 cm**-1
35: 1289.70 cm**-1
36: 1316.64 cm**-1
37: 1326.57 cm**-1
38: 1338.42 cm**-1
39: 1350.56 cm**-1
40: 1374.53 cm**-1
41: 1415.86 cm**-1
42: 1418.85 cm**-1
43: 1481.73 cm**-1
44: 1488.26 cm**-1
45: 1495.81 cm**-1
46: 1496.72 cm**-1
47: 1509.12 cm**-1
48: 1570.31 cm**-1
49: 1628.79 cm**-1
50: 3019.05 cm**-1
51: 3022.49 cm**-1
52: 3028.30 cm**-1
53: 3035.88 cm**-1
54: 3048.98 cm**-1
55: 3075.77 cm**-1
56: 3094.40 cm**-1
57: 3101.04 cm**-1
58: 3101.97 cm**-1
59: 3133.64 cm**-1
60: 3159.19 cm**-1
61: 3175.53 cm**-1
62: 3695.28 cm**-1

GIBBS FREE ENERGY

Total enthalpy ... -349.21225871 Eh
Total entropy correction ... -0.04554981 Eh -28.58 kcal/mol

Final Gibbs free energy ... -349.25780852

2-HEPTANONE C₇H₁₄O

CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.561790	0.960400	-0.005870
C	-4.207470	1.618790	0.030200
H	-5.759660	0.587770	-1.013550
H	-6.330590	1.688810	0.267800
H	-5.594540	0.138640	0.713710
C	-3.003130	0.693410	-0.030160
C	-1.685470	1.464290	0.018610
H	-3.066820	0.113790	-0.957560
H	-3.064300	0.004150	0.819300
C	-0.470590	0.535830	-0.024190
H	-1.650340	2.070120	0.932810
H	-1.640290	2.164850	-0.824660
C	0.828970	1.340960	0.035680
H	-0.493480	-0.061840	-0.943460
H	-0.510150	-0.164280	0.819100
C	2.056520	0.445470	-0.000520
H	0.851150	1.940240	0.953470
H	0.871260	2.040080	-0.807760
H	2.061360	-0.250470	0.844220
H	2.966490	1.051770	0.054840
H	2.092430	-0.135510	-0.927380
O	-4.104440	2.844660	0.073560

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.578732	0.932425	-0.078561
C	-4.246411	1.634434	0.106799
H	-5.668395	0.585256	-1.113520
H	-6.395803	1.618767	0.141654
H	-5.647912	0.048722	0.562875
C	-3.008261	0.752921	0.038488
C	-1.685381	1.514334	0.044662
H	-3.090896	0.114117	-0.850917
H	-3.059580	0.060665	0.891040
C	-0.469345	0.585576	0.003638
H	-1.640761	2.149505	0.934680
H	-1.660242	2.198123	-0.810640
C	0.865423	1.336766	0.001961
H	-0.523447	-0.053313	-0.888250
H	-0.498384	-0.094560	0.865681
C	2.079422	0.405015	-0.030385
H	0.918096	1.977619	0.890441
H	0.896672	2.011624	-0.862085
H	2.090828	-0.258237	0.840731
H	3.016612	0.968590	-0.031102
H	2.069869	-0.225852	-0.925251
O	-4.178251	2.829431	0.296251

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm**-1
1:	0.00	cm**-1
2:	0.00	cm**-1
3:	0.00	cm**-1
4:	0.00	cm**-1
5:	0.00	cm**-1
6:	34.08	cm**-1
7:	55.26	cm**-1
8:	86.87	cm**-1
9:	95.99	cm**-1
10:	118.46	cm**-1
11:	132.75	cm**-1

12: 225.16 cm**⁻¹
 13: 244.15 cm**⁻¹
 14: 288.73 cm**⁻¹
 15: 401.93 cm**⁻¹
 16: 459.99 cm**⁻¹
 17: 477.38 cm**⁻¹
 18: 601.43 cm**⁻¹
 19: 723.69 cm**⁻¹
 20: 747.76 cm**⁻¹
 21: 818.32 cm**⁻¹
 22: 827.83 cm**⁻¹
 23: 909.17 cm**⁻¹
 24: 931.21 cm**⁻¹
 25: 942.96 cm**⁻¹
 26: 1009.22 cm**⁻¹
 27: 1025.55 cm**⁻¹
 28: 1061.58 cm**⁻¹
 29: 1067.83 cm**⁻¹
 30: 1133.56 cm**⁻¹
 31: 1147.67 cm**⁻¹
 32: 1178.12 cm**⁻¹
 33: 1225.46 cm**⁻¹
 34: 1272.42 cm**⁻¹
 35: 1291.34 cm**⁻¹
 36: 1328.21 cm**⁻¹
 37: 1333.59 cm**⁻¹
 38: 1342.71 cm**⁻¹
 39: 1383.04 cm**⁻¹
 40: 1393.65 cm**⁻¹
 41: 1403.09 cm**⁻¹
 42: 1413.08 cm**⁻¹
 43: 1451.40 cm**⁻¹
 44: 1466.20 cm**⁻¹
 45: 1476.84 cm**⁻¹
 46: 1485.42 cm**⁻¹
 47: 1489.55 cm**⁻¹
 48: 1499.08 cm**⁻¹
 49: 1500.66 cm**⁻¹
 50: 1511.45 cm**⁻¹
 51: 1781.54 cm**⁻¹
 52: 2986.94 cm**⁻¹
 53: 2996.28 cm**⁻¹
 54: 3005.98 cm**⁻¹
 55: 3007.95 cm**⁻¹
 56: 3014.98 cm**⁻¹
 57: 3019.92 cm**⁻¹
 58: 3026.57 cm**⁻¹
 59: 3030.65 cm**⁻¹
 60: 3036.24 cm**⁻¹
 61: 3069.07 cm**⁻¹
 62: 3075.42 cm**⁻¹
 63: 3081.24 cm**⁻¹
 64: 3082.36 cm**⁻¹
 65: 3134.65 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-350.09866777 Eh	
Total entropy correction	...	-0.04713281 Eh	-29.58 kcal/mol

Final Gibbs free energy	...	-350.14580057	

PROTONATED 2-HEPTANONE C₇H₁₄O⁺
CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.578810	0.933140	-0.073220
C	-4.245790	1.633830	0.109740
H	-5.675040	0.597860	-1.111620
H	-6.394890	1.616500	0.159450
H	-5.642970	0.041780	0.557970
C	-3.008270	0.752540	0.031860
C	-1.685360	1.513550	0.040270
H	-3.094380	0.121010	-0.862500
H	-3.057650	0.052530	0.878160
C	-0.469050	0.585110	0.002750
H	-1.643050	2.149800	0.929640
H	-1.658410	2.196710	-0.815530
C	0.865320	1.336980	-0.000580
H	-0.522350	-0.056900	-0.886950
H	-0.498430	-0.092360	0.866880
C	2.079460	0.405520	-0.024510
H	0.915660	1.983670	0.883800
H	0.898220	2.006500	-0.868720
H	2.089180	-0.252490	0.850610
H	3.016600	0.969210	-0.026670
H	2.072050	-0.230960	-0.915430
O	-4.176890	2.828390	0.302800
H	-5.023640	3.793280	0.238820

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.564783	0.984957	-0.168321
C	-4.245738	1.582681	0.118842
H	-5.662215	0.936066	-1.263628
H	-6.397064	1.572158	0.225880
H	-5.613304	-0.043059	0.195486
C	-3.004971	0.796986	0.115257
C	-1.679280	1.561900	0.039523
H	-3.100209	0.029566	-0.664710
H	-3.064820	0.213190	1.054986
C	-0.481940	0.605593	0.041393
H	-1.605846	2.254615	0.882487
H	-1.668004	2.171134	-0.870398
C	0.858438	1.343415	-0.041888
H	-0.566097	-0.090597	-0.802586
H	-0.504488	-0.007446	0.951325
C	2.055931	0.391040	-0.042511
H	0.939840	2.038460	0.802030
H	0.875688	1.957991	-0.949726
H	2.084317	-0.211880	0.870016
H	2.995730	0.943888	-0.103618
H	2.018256	-0.294079	-0.894756
O	-4.130978	2.832321	0.372483
H	-4.976953	3.316299	0.399455

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	41.67	cm** ⁻¹
7:	55.11	cm** ⁻¹
8:	95.65	cm** ⁻¹
9:	104.58	cm** ⁻¹

10: 131.35 cm**-1
 11: 144.17 cm**-1
 12: 224.48 cm**-1
 13: 243.49 cm**-1
 14: 292.88 cm**-1
 15: 401.13 cm**-1
 16: 447.55 cm**-1
 17: 469.10 cm**-1
 18: 584.77 cm**-1
 19: 675.19 cm**-1
 20: 736.24 cm**-1
 21: 763.04 cm**-1
 22: 832.00 cm**-1
 23: 855.97 cm**-1
 24: 914.37 cm**-1
 25: 949.82 cm**-1
 26: 975.94 cm**-1
 27: 1004.13 cm**-1
 28: 1028.06 cm**-1
 29: 1043.76 cm**-1
 30: 1063.40 cm**-1
 31: 1112.02 cm**-1
 32: 1131.82 cm**-1
 33: 1150.84 cm**-1
 34: 1217.58 cm**-1
 35: 1253.21 cm**-1
 36: 1281.01 cm**-1
 37: 1317.84 cm**-1
 38: 1332.93 cm**-1
 39: 1339.06 cm**-1
 40: 1374.23 cm**-1
 41: 1379.13 cm**-1
 42: 1386.50 cm**-1
 43: 1401.99 cm**-1
 44: 1420.88 cm**-1
 45: 1421.56 cm**-1
 46: 1467.21 cm**-1
 47: 1483.54 cm**-1
 48: 1487.23 cm**-1
 49: 1490.05 cm**-1
 50: 1500.16 cm**-1
 51: 1501.37 cm**-1
 52: 1511.65 cm**-1
 53: 1563.48 cm**-1
 54: 2939.39 cm**-1
 55: 2999.57 cm**-1
 56: 3004.26 cm**-1
 57: 3012.56 cm**-1
 58: 3023.40 cm**-1
 59: 3026.18 cm**-1
 60: 3027.86 cm**-1
 61: 3036.50 cm**-1
 62: 3047.79 cm**-1
 63: 3082.08 cm**-1
 64: 3083.81 cm**-1
 65: 3087.39 cm**-1
 66: 3101.01 cm**-1
 67: 3134.41 cm**-1
 68: 3672.72 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-350.41296491 Eh	
Total entropy correction	...	-0.04707257 Eh	-29.54 kcal/mol

Final Gibbs free energy ... -350.46003747 E

HEPTANAL C₇H₁₄O

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	3.386700	1.080600	-0.023500
C	-0.535400	-0.654400	0.008600
C	-1.703400	0.333900	0.018200
C	0.810400	0.076500	0.033700
C	-3.047000	-0.392700	-0.037700
C	1.994200	-0.885000	-0.005600
C	-4.211000	0.584500	0.004900
C	3.305300	-0.143400	0.001500
H	-0.607200	-1.321000	0.876500
H	-0.592800	-1.282700	-0.888500
H	-1.619000	1.013400	-0.838700
H	-1.654400	0.949400	0.924700
H	0.870300	0.698500	0.935900
H	0.865400	0.761200	-0.822400
H	-3.110000	-0.989200	-0.955300
H	-3.130500	-1.086700	0.806900
H	1.963200	-1.502300	-0.909400
H	1.979100	-1.547100	0.866300
H	-5.161600	0.043700	-0.037100
H	-4.174900	1.274600	-0.844100
H	-4.195600	1.173100	0.927600
H	4.209900	-0.774600	0.018800

FINAL GEOMETRY OPTIMIZATION CYCLE

O	3.558228	1.013463	0.038173
C	-0.523375	-0.614499	-0.011984
C	-1.725970	0.332077	0.012519
C	0.821405	0.116839	0.018002
C	-3.074417	-0.393220	-0.022512
C	2.011186	-0.838326	-0.004043
C	-4.270323	0.561279	0.009398
C	3.365729	-0.177729	0.018169
H	-0.585635	-1.300364	0.843424
H	-0.577160	-1.244455	-0.909906
H	-1.663289	1.020647	-0.840228
H	-1.675337	0.959219	0.912170
H	0.883182	0.746990	0.911512
H	0.893126	0.801023	-0.833871
H	-3.125807	-1.015043	-0.924961
H	-3.133938	-1.084977	0.826956
H	1.989749	-1.486083	-0.893390
H	1.982830	-1.536966	0.845380
H	-5.218713	0.017360	-0.019159
H	-4.252733	1.244314	-0.846095
H	-4.263889	1.171793	0.918154
H	4.226850	-0.883043	0.013592

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	49.17	cm** ⁻¹
7:	65.35	cm** ⁻¹
8:	84.02	cm** ⁻¹
9:	121.04	cm** ⁻¹
10:	137.73	cm** ⁻¹

11: 179.34 cm**⁻¹
 12: 191.27 cm**⁻¹
 13: 244.00 cm**⁻¹
 14: 274.03 cm**⁻¹
 15: 382.05 cm**⁻¹
 16: 454.64 cm**⁻¹
 17: 667.30 cm**⁻¹
 18: 703.64 cm**⁻¹
 19: 733.35 cm**⁻¹
 20: 761.15 cm**⁻¹
 21: 840.65 cm**⁻¹
 22: 881.96 cm**⁻¹
 23: 912.42 cm**⁻¹
 24: 933.97 cm**⁻¹
 25: 1013.33 cm**⁻¹
 26: 1016.62 cm**⁻¹
 27: 1052.78 cm**⁻¹
 28: 1063.39 cm**⁻¹
 29: 1072.90 cm**⁻¹
 30: 1138.59 cm**⁻¹
 31: 1160.05 cm**⁻¹
 32: 1220.32 cm**⁻¹
 33: 1254.67 cm**⁻¹
 34: 1273.91 cm**⁻¹
 35: 1314.40 cm**⁻¹
 36: 1316.62 cm**⁻¹
 37: 1332.17 cm**⁻¹
 38: 1336.25 cm**⁻¹
 39: 1368.69 cm**⁻¹
 40: 1398.87 cm**⁻¹
 41: 1403.35 cm**⁻¹
 42: 1413.28 cm**⁻¹
 43: 1413.78 cm**⁻¹
 44: 1447.39 cm**⁻¹
 45: 1485.42 cm**⁻¹
 46: 1486.05 cm**⁻¹
 47: 1493.95 cm**⁻¹
 48: 1499.03 cm**⁻¹
 49: 1503.90 cm**⁻¹
 50: 1512.66 cm**⁻¹
 51: 1800.10 cm**⁻¹
 52: 2859.45 cm**⁻¹
 53: 2986.87 cm**⁻¹
 54: 2990.40 cm**⁻¹
 55: 2994.28 cm**⁻¹
 56: 3004.88 cm**⁻¹
 57: 3006.01 cm**⁻¹
 58: 3007.14 cm**⁻¹
 59: 3015.82 cm**⁻¹
 60: 3019.63 cm**⁻¹
 61: 3030.31 cm**⁻¹
 62: 3041.49 cm**⁻¹
 63: 3067.00 cm**⁻¹
 64: 3075.87 cm**⁻¹
 65: 3081.02 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-350.08692491 Eh	
Total entropy correction	...	-0.04646215 Eh	-29.16 kcal/mol

Final Gibbs free energy	...	-350.13338706	

PROTONATED HEPTANAL C₇H₁₄O⁺
CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	3.557980	1.013590	0.041210
C	-0.523470	-0.614590	-0.012640
C	-1.725960	0.332100	0.012870
C	0.821400	0.116640	0.017520
C	-3.074460	-0.393200	-0.021740
C	2.011270	-0.838330	-0.004210
C	-4.270380	0.561370	0.009120
C	3.365790	-0.177550	0.018520
H	-0.585500	-1.301170	0.842210
H	-0.577490	-1.243750	-0.911090
H	-1.663740	1.020960	-0.839670
H	-1.674820	0.958910	0.912710
H	0.883050	0.747060	0.910830
H	0.893250	0.800650	-0.834510
H	-3.125680	-1.015870	-0.923600
H	-3.134100	-1.084180	0.828350
H	1.990310	-1.486560	-0.893210
H	1.982960	-1.536730	0.845480
H	-5.218810	0.017490	-0.018980
H	-4.252710	1.243540	-0.847050
H	-4.264070	1.172810	0.917250
H	4.226890	-0.882890	0.011960
H	3.374950	2.132280	0.087140

FINAL GEOMETRY OPTIMIZATION CYCLE

O	3.591834	1.051215	0.055955
C	-0.497288	-0.587033	-0.013467
C	-1.700261	0.359065	0.012944
C	0.843309	0.164196	0.018148
C	-3.041749	-0.381801	-0.017854
C	2.037579	-0.791895	-0.004482
C	-4.241021	0.568061	0.009085
C	3.363180	-0.192386	0.021294
H	-0.544527	-1.269540	0.843256
H	-0.536748	-1.210535	-0.914395
H	-1.645006	1.043681	-0.842987
H	-1.652356	0.984635	0.913348
H	0.878001	0.781307	0.926059
H	0.888423	0.837750	-0.848199
H	-3.087449	-1.007049	-0.917327
H	-3.094673	-1.066916	0.836451
H	2.037101	-1.461407	-0.885073
H	2.025378	-1.517367	0.830036
H	-5.181749	0.013762	-0.015159
H	-4.231754	1.243191	-0.851984
H	-4.240977	1.182010	0.914796
H	4.273818	-0.793648	0.011215
H	2.773593	1.593284	0.066811

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	45.22	cm** ⁻¹
7:	63.87	cm** ⁻¹
8:	81.73	cm** ⁻¹
9:	115.16	cm** ⁻¹

10: 135.48 cm**-1
 11: 180.98 cm**-1
 12: 187.27 cm**-1
 13: 243.95 cm**-1
 14: 271.27 cm**-1
 15: 375.90 cm**-1
 16: 451.51 cm**-1
 17: 560.70 cm**-1
 18: 653.39 cm**-1
 19: 737.37 cm**-1
 20: 757.96 cm**-1
 21: 809.43 cm**-1
 22: 892.83 cm**-1
 23: 895.10 cm**-1
 24: 930.22 cm**-1
 25: 989.80 cm**-1
 26: 1008.77 cm**-1
 27: 1036.51 cm**-1
 28: 1044.13 cm**-1
 29: 1051.04 cm**-1
 30: 1064.67 cm**-1
 31: 1133.11 cm**-1
 32: 1156.76 cm**-1
 33: 1218.41 cm**-1
 34: 1227.14 cm**-1
 35: 1264.70 cm**-1
 36: 1270.66 cm**-1
 37: 1312.81 cm**-1
 38: 1323.83 cm**-1
 39: 1338.23 cm**-1
 40: 1341.02 cm**-1
 41: 1344.10 cm**-1
 42: 1376.34 cm**-1
 43: 1396.84 cm**-1
 44: 1402.17 cm**-1
 45: 1420.92 cm**-1
 46: 1455.95 cm**-1
 47: 1486.19 cm**-1
 48: 1487.35 cm**-1
 49: 1494.49 cm**-1
 50: 1501.31 cm**-1
 51: 1503.21 cm**-1
 52: 1512.72 cm**-1
 53: 1604.94 cm**-1
 54: 2958.87 cm**-1
 55: 2962.13 cm**-1
 56: 2990.07 cm**-1
 57: 2998.10 cm**-1
 58: 3009.80 cm**-1
 59: 3017.29 cm**-1
 60: 3020.24 cm**-1
 61: 3025.24 cm**-1
 62: 3026.74 cm**-1
 63: 3043.92 cm**-1
 64: 3062.19 cm**-1
 65: 3085.70 cm**-1
 66: 3099.84 cm**-1
 67: 3148.46 cm**-1
 68: 3577.35 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-350.38807281 Eh	
Total entropy correction	...	-0.04681745 Eh	-29.38 kcal/mol

Final Gibbs free energy ... -350.43489026

2,3-HEPTANEDIONE C₇H₁₂O₂
CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.083490	2.594280	-0.079010
C	-4.809110	1.177990	0.328010
H	-6.133200	2.831280	0.115710
H	-4.898670	2.718590	-1.148690
H	-4.450920	3.275180	0.494860
C	-3.523950	0.560940	-0.199550
C	-2.266980	1.372410	0.013250
C	-1.010320	0.510080	-0.076100
H	-2.316440	1.837940	1.003850
H	-2.241640	2.163660	-0.743760
C	0.253510	1.352660	0.086490
H	-0.980820	-0.011170	-1.040500
H	-1.044470	-0.265490	0.698840
C	1.506530	0.493760	0.039290
H	0.224140	1.893090	1.039390
H	0.302790	2.103670	-0.710310
H	1.512390	-0.235390	0.855450
H	2.399290	1.119070	0.136970
H	1.575120	-0.050390	-0.907750
O	-5.525690	0.538820	1.085740
O	-3.574520	-0.501660	-0.803590

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.871950	1.915822	-0.421203
C	-4.566358	2.090598	0.305418
H	-6.657465	2.458372	0.102572
H	-6.122220	0.853947	-0.494939
H	-5.778654	2.278468	-1.449010
C	-3.337785	1.352451	-0.297336
C	-2.021658	1.549686	0.409605
C	-0.863813	0.769534	-0.205721
H	-2.168304	1.293915	1.466455
H	-1.817023	2.628452	0.423635
C	0.460345	1.007349	0.525916
H	-0.759083	1.046009	-1.260296
H	-1.102811	-0.299520	-0.201165
C	1.624844	0.226186	-0.087652
H	0.348653	0.730228	1.581459
H	0.692902	2.079450	0.516215
H	1.434266	-0.851378	-0.060287
H	2.558504	0.413052	0.449956
H	1.780174	0.507519	-1.134013
O	-4.429225	2.758122	1.305610
O	-3.489789	0.671059	-1.286626

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	30.91	cm** ⁻¹
7:	42.05	cm** ⁻¹
8:	78.59	cm** ⁻¹
9:	96.57	cm** ⁻¹
10:	106.72	cm** ⁻¹
11:	125.67	cm** ⁻¹
12:	220.54	cm** ⁻¹
13:	242.05	cm** ⁻¹
14:	284.18	cm** ⁻¹

15: 326.92 cm**-1
 16: 351.33 cm**-1
 17: 431.25 cm**-1
 18: 532.48 cm**-1
 19: 590.41 cm**-1
 20: 594.23 cm**-1
 21: 731.92 cm**-1
 22: 781.03 cm**-1
 23: 793.03 cm**-1
 24: 910.32 cm**-1
 25: 919.67 cm**-1
 26: 924.07 cm**-1
 27: 1009.27 cm**-1
 28: 1024.97 cm**-1
 29: 1062.41 cm**-1
 30: 1071.90 cm**-1
 31: 1115.55 cm**-1
 32: 1134.44 cm**-1
 33: 1227.63 cm**-1
 34: 1232.31 cm**-1
 35: 1299.79 cm**-1
 36: 1305.05 cm**-1
 37: 1330.93 cm**-1
 38: 1375.81 cm**-1
 39: 1389.58 cm**-1
 40: 1406.73 cm**-1
 41: 1415.27 cm**-1
 42: 1438.98 cm**-1
 43: 1456.49 cm**-1
 44: 1458.30 cm**-1
 45: 1487.36 cm**-1
 46: 1495.76 cm**-1
 47: 1499.12 cm**-1
 48: 1510.20 cm**-1
 49: 1777.02 cm**-1
 50: 1782.45 cm**-1
 51: 3001.81 cm**-1
 52: 3014.83 cm**-1
 53: 3017.72 cm**-1
 54: 3023.16 cm**-1
 55: 3027.75 cm**-1
 56: 3035.75 cm**-1
 57: 3039.86 cm**-1
 58: 3063.73 cm**-1
 59: 3079.38 cm**-1
 60: 3083.93 cm**-1
 61: 3095.17 cm**-1
 62: 3146.47 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-424.12343719 Eh	
Total entropy correction	...	-0.04864324 Eh	-30.52 kcal/mol

Final Gibbs free energy	...	-424.17208043	

PROTONATED 2,3-HEPTANEDIONE C₇H₁₂O₂⁺
CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.872320	1.914130	-0.419470
C	-4.565910	2.091980	0.304370
H	-6.657570	2.457630	0.103680
H	-6.121590	0.851790	-0.489410
H	-5.780620	2.273470	-1.448560
C	-3.336770	1.355890	-0.300090
C	-2.021590	1.549790	0.409070
C	-0.863560	0.770480	-0.206960
H	-2.170130	1.290220	1.464670
H	-1.816290	2.628370	0.427290
C	0.460140	1.007740	0.525450
H	-0.758720	1.047730	-1.261320
H	-1.102690	-0.298550	-0.203050
C	1.624460	0.225090	-0.086420
H	0.347390	0.731480	1.581130
H	0.693650	2.079630	0.515320
H	1.433490	-0.852360	-0.057220
H	2.558070	0.412490	0.451100
H	1.780200	0.504450	-1.133250
O	-4.428200	2.759960	1.304320
O	-3.487890	0.677910	-1.292060
H	-6.279760	4.274290	0.952310

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.901595	1.696421	-0.136427
C	-4.581296	2.308235	0.008617
H	-6.725011	2.357813	0.136781
H	-5.928775	0.784777	0.478922
H	-5.999652	1.343115	-1.170707
C	-3.310231	1.590360	-0.498404
C	-2.084269	1.606323	0.348919
C	-0.891891	0.883186	-0.282411
H	-2.352164	1.165316	1.322551
H	-1.848389	2.656155	0.575740
C	0.342661	0.915156	0.625897
H	-0.662040	1.348419	-1.245779
H	-1.169735	-0.152972	-0.500047
C	1.543181	0.205031	-0.003277
H	0.099770	0.447443	1.587544
H	0.604754	1.956980	0.845761
H	1.319378	-0.845770	-0.208579
H	2.407761	0.236931	0.663039
H	1.832073	0.676872	-0.946754
O	-4.388432	3.486471	0.450947
O	-3.469256	1.108814	-1.590349
H	-5.203051	3.978536	0.678916

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	22.21	cm** ⁻¹
7:	43.93	cm** ⁻¹
8:	75.62	cm** ⁻¹
9:	92.51	cm** ⁻¹
10:	118.08	cm** ⁻¹
11:	126.03	cm** ⁻¹

12: 203.87 cm**⁻¹
 13: 239.99 cm**⁻¹
 14: 254.85 cm**⁻¹
 15: 293.96 cm**⁻¹
 16: 326.32 cm**⁻¹
 17: 416.66 cm**⁻¹
 18: 546.14 cm**⁻¹
 19: 559.95 cm**⁻¹
 20: 578.82 cm**⁻¹
 21: 727.01 cm**⁻¹
 22: 746.20 cm**⁻¹
 23: 780.00 cm**⁻¹
 24: 805.21 cm**⁻¹
 25: 915.63 cm**⁻¹
 26: 924.41 cm**⁻¹
 27: 937.47 cm**⁻¹
 28: 993.57 cm**⁻¹
 29: 1025.35 cm**⁻¹
 30: 1057.46 cm**⁻¹
 31: 1067.95 cm**⁻¹
 32: 1117.88 cm**⁻¹
 33: 1123.98 cm**⁻¹
 34: 1141.64 cm**⁻¹
 35: 1228.15 cm**⁻¹
 36: 1290.66 cm**⁻¹
 37: 1305.29 cm**⁻¹
 38: 1334.46 cm**⁻¹
 39: 1343.64 cm**⁻¹
 40: 1367.14 cm**⁻¹
 41: 1397.55 cm**⁻¹
 42: 1407.62 cm**⁻¹
 43: 1415.10 cm**⁻¹
 44: 1421.91 cm**⁻¹
 45: 1430.49 cm**⁻¹
 46: 1444.05 cm**⁻¹
 47: 1487.56 cm**⁻¹
 48: 1494.18 cm**⁻¹
 49: 1500.38 cm**⁻¹
 50: 1509.61 cm**⁻¹
 51: 1568.61 cm**⁻¹
 52: 1794.64 cm**⁻¹
 53: 2980.59 cm**⁻¹
 54: 3002.89 cm**⁻¹
 55: 3008.09 cm**⁻¹
 56: 3013.90 cm**⁻¹
 57: 3028.68 cm**⁻¹
 58: 3034.15 cm**⁻¹
 59: 3038.35 cm**⁻¹
 60: 3053.39 cm**⁻¹
 61: 3077.27 cm**⁻¹
 62: 3091.95 cm**⁻¹
 63: 3103.44 cm**⁻¹
 64: 3130.46 cm**⁻¹
 65: 3618.24 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-424.41651267 Eh	
Total entropy correction	...	-0.04929206 Eh	-30.93 kcal/mol

Final Gibbs free energy	...	-424.46580473	

MENTHONE C₁₀H₁₈O

CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	0.014400	-2.244100	0.654700
C	-0.673500	0.056800	0.637600
C	0.193200	1.301000	0.847400
C	2.020100	0.377100	-0.674900
C	1.138600	1.583300	-0.320700
C	-1.803800	0.284600	-0.361200
C	1.170700	-0.869300	-0.931000
C	0.182000	-1.116600	0.189600
C	3.082800	0.111800	0.396000
C	-2.668900	-0.967900	-0.490600
C	-2.655500	1.483300	0.053200
H	-1.101100	-0.210700	1.613800
H	0.803700	1.139000	1.745900
H	-0.396300	2.193200	1.075600
H	2.556800	0.616200	-1.602300
H	0.551300	1.871500	-1.201200
H	1.769100	2.446600	-0.076100
H	-1.398800	0.496400	-1.358600
H	1.809000	-1.753000	-1.043200
H	0.601300	-0.758700	-1.860600
H	3.683900	1.009300	0.575900
H	2.644600	-0.199600	1.349000
H	3.763300	-0.682500	0.070300
H	-3.059100	-1.286600	0.482100
H	-3.526300	-0.778800	-1.146300
H	-2.115900	-1.803300	-0.930700
H	-2.958700	1.419600	1.103700
H	-3.568500	1.534600	-0.551100
H	-2.132700	2.430900	-0.105600

FINAL GEOMETRY OPTIMIZATION CYCLE

O	0.179902	-2.126648	0.932919
C	-0.676028	0.104205	0.678276
C	0.250066	1.329419	0.873296
C	2.015202	0.353245	-0.696850
C	1.159957	1.582807	-0.335989
C	-1.809716	0.327927	-0.361468
C	1.104491	-0.883458	-0.895505
C	0.192199	-1.090937	0.300327
C	3.104297	0.071571	0.346882
C	-2.607176	-0.963167	-0.592651
C	-2.751292	1.456927	0.077722
H	-1.148358	-0.148270	1.633473
H	0.863428	1.158502	1.763839
H	-0.346389	2.218507	1.090730
H	2.513252	0.554122	-1.652147
H	0.552866	1.866223	-1.203204
H	1.815312	2.435665	-0.130044
H	-1.357204	0.621400	-1.315931
H	1.689503	-1.792134	-1.049973
H	0.477616	-0.728377	-1.781867
H	3.745563	0.947119	0.484848
H	2.683195	-0.193309	1.320705
H	3.736889	-0.763093	0.032245
H	-3.053552	-1.315213	0.343093
H	-3.416586	-0.792880	-1.308131
H	-1.984374	-1.773519	-0.979873
H	-3.189944	1.236919	1.057053
H	-3.572448	1.568325	-0.636217
H	-2.244971	2.422221	0.145143

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm**-1
1:	0.00	cm**-1
2:	0.00	cm**-1
3:	0.00	cm**-1
4:	0.00	cm**-1
5:	0.00	cm**-1
6:	46.97	cm**-1
7:	78.69	cm**-1
8:	103.73	cm**-1
9:	154.01	cm**-1
10:	182.88	cm**-1
11:	215.82	cm**-1
12:	223.91	cm**-1
13:	234.53	cm**-1
14:	321.88	cm**-1
15:	332.04	cm**-1
16:	366.40	cm**-1
17:	379.64	cm**-1
18:	392.93	cm**-1
19:	429.79	cm**-1
20:	448.81	cm**-1
21:	518.07	cm**-1
22:	552.42	cm**-1
23:	588.98	cm**-1
24:	702.27	cm**-1
25:	750.06	cm**-1
26:	806.79	cm**-1
27:	820.80	cm**-1
28:	866.83	cm**-1
29:	904.14	cm**-1
30:	926.41	cm**-1
31:	933.52	cm**-1
32:	959.74	cm**-1
33:	967.04	cm**-1
34:	972.81	cm**-1
35:	993.97	cm**-1
36:	1019.61	cm**-1
37:	1060.00	cm**-1
38:	1071.87	cm**-1
39:	1097.90	cm**-1
40:	1127.45	cm**-1
41:	1154.25	cm**-1
42:	1173.42	cm**-1
43:	1185.67	cm**-1
44:	1217.62	cm**-1
45:	1244.69	cm**-1
46:	1266.20	cm**-1
47:	1292.42	cm**-1
48:	1299.20	cm**-1
49:	1322.81	cm**-1
50:	1354.28	cm**-1
51:	1356.98	cm**-1
52:	1367.54	cm**-1
53:	1373.15	cm**-1
54:	1377.53	cm**-1
55:	1393.95	cm**-1
56:	1404.17	cm**-1
57:	1418.62	cm**-1
58:	1426.15	cm**-1
59:	1473.31	cm**-1
60:	1486.56	cm**-1
61:	1486.93	cm**-1
62:	1493.05	cm**-1
63:	1498.85	cm**-1

64: 1503.26 cm**⁻¹
 65: 1504.90 cm**⁻¹
 66: 1508.99 cm**⁻¹
 67: 1519.50 cm**⁻¹
 68: 1772.94 cm**⁻¹
 69: 3005.09 cm**⁻¹
 70: 3012.26 cm**⁻¹
 71: 3017.12 cm**⁻¹
 72: 3018.06 cm**⁻¹
 73: 3021.63 cm**⁻¹
 74: 3022.12 cm**⁻¹
 75: 3028.36 cm**⁻¹
 76: 3032.01 cm**⁻¹
 77: 3041.15 cm**⁻¹
 78: 3053.56 cm**⁻¹
 79: 3070.25 cm**⁻¹
 80: 3076.09 cm**⁻¹
 81: 3084.24 cm**⁻¹
 82: 3084.50 cm**⁻¹
 83: 3088.74 cm**⁻¹
 84: 3090.01 cm**⁻¹
 85: 3091.63 cm**⁻¹
 86: 3095.31 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-466.73107800 Eh	
Total entropy correction	...	-0.04933087 Eh	-30.96 kcal/mol

Final Gibbs free energy	...	-466.78040887 Eh	

PROTONATED MENTHONE C₁₀H₁₈O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	0.369860	-2.093630	0.847490
C	-0.622210	0.068230	0.657380
C	0.283170	1.306840	0.896100
C	2.045990	0.420040	-0.748540
C	1.159450	1.627690	-0.338600
C	-1.772380	0.306320	-0.378840
C	1.166930	-0.824230	-0.995060
C	0.294040	-1.053530	0.211370
C	3.137300	0.125090	0.297910
C	-2.599350	-0.977530	-0.577230
C	-2.724010	1.432630	0.061550
H	-1.106490	-0.205440	1.622020
H	0.949030	1.097910	1.758980
H	-0.309390	2.194080	1.192070
H	2.578850	0.674810	-1.691030
H	0.500350	1.900260	-1.189240
H	1.801350	2.510070	-0.127470
H	-1.354800	0.588910	-1.367050
H	1.799190	-1.711240	-1.218590
H	0.515980	-0.648830	-1.876710
H	3.773690	1.022890	0.447470
H	2.715360	-0.179750	1.276680
H	3.787500	-0.701340	-0.060190
H	-3.059650	-1.300380	0.381380
H	-3.407500	-0.804870	-1.320010
H	-1.966560	-1.802830	-0.964920
H	-3.176400	1.201210	1.049810
H	-3.540640	1.555410	-0.681930
H	-2.202700	2.407950	0.119240
H	1.350590	-2.336010	0.523550

FINAL GEOMETRY OPTIMIZATION CYCLE

O	0.306050	-2.026685	0.947010
C	-0.607606	0.118876	0.652267
C	0.305607	1.378388	0.842898
C	2.070442	0.442835	-0.744128
C	1.198011	1.651560	-0.369019
C	-1.776899	0.329823	-0.381756
C	1.142244	-0.813373	-0.961496
C	0.272288	-0.971232	0.212947
C	3.171074	0.136574	0.275707
C	-2.500081	-0.994433	-0.657240
C	-2.754066	1.383509	0.146534
H	-1.053074	-0.165371	1.609124
H	0.911849	1.230245	1.739990
H	-0.343955	2.228098	1.051824
H	2.536397	0.628289	-1.714941
H	0.590251	1.948589	-1.228814
H	1.849271	2.502022	-0.149667
H	-1.338384	0.695231	-1.315913
H	1.731511	-1.713482	-1.158269
H	0.504543	-0.617028	-1.829849
H	3.839803	0.994153	0.374381
H	2.775377	-0.084255	1.272276
H	3.778527	-0.715882	-0.040014
H	-2.902590	-1.424156	0.265153
H	-3.337067	-0.833865	-1.339065
H	-1.850374	-1.745084	-1.121615
H	-3.176581	1.081064	1.109227
H	-3.581685	1.495960	-0.557706
H	-2.295227	2.366163	0.264393
H	0.920895	-2.705802	0.613351

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	50.78	cm** ⁻¹
7:	71.44	cm** ⁻¹
8:	91.85	cm** ⁻¹
9:	145.45	cm** ⁻¹
10:	179.58	cm** ⁻¹
11:	216.89	cm** ⁻¹
12:	233.26	cm** ⁻¹
13:	250.12	cm** ⁻¹
14:	306.19	cm** ⁻¹
15:	324.43	cm** ⁻¹
16:	361.94	cm** ⁻¹
17:	373.15	cm** ⁻¹
18:	389.54	cm** ⁻¹
19:	423.76	cm** ⁻¹
20:	446.33	cm** ⁻¹
21:	491.42	cm** ⁻¹
22:	537.31	cm** ⁻¹
23:	587.48	cm** ⁻¹
24:	705.37	cm** ⁻¹
25:	729.30	cm** ⁻¹
26:	766.07	cm** ⁻¹
27:	803.32	cm** ⁻¹
28:	835.54	cm** ⁻¹
29:	861.42	cm** ⁻¹
30:	891.29	cm** ⁻¹
31:	907.47	cm** ⁻¹
32:	932.86	cm** ⁻¹
33:	938.84	cm** ⁻¹
34:	957.14	cm** ⁻¹
35:	966.25	cm** ⁻¹
36:	991.37	cm** ⁻¹
37:	1015.99	cm** ⁻¹
38:	1049.13	cm** ⁻¹
39:	1069.86	cm** ⁻¹
40:	1097.40	cm** ⁻¹
41:	1121.84	cm** ⁻¹
42:	1140.40	cm** ⁻¹
43:	1149.71	cm** ⁻¹
44:	1179.56	cm** ⁻¹
45:	1184.20	cm** ⁻¹
46:	1199.52	cm** ⁻¹
47:	1241.26	cm** ⁻¹
48:	1256.55	cm** ⁻¹
49:	1292.44	cm** ⁻¹
50:	1322.17	cm** ⁻¹
51:	1342.50	cm** ⁻¹
52:	1347.79	cm** ⁻¹
53:	1353.18	cm** ⁻¹
54:	1361.57	cm** ⁻¹
55:	1364.20	cm** ⁻¹
56:	1395.18	cm** ⁻¹
57:	1413.31	cm** ⁻¹
58:	1427.76	cm** ⁻¹
59:	1433.78	cm** ⁻¹
60:	1458.65	cm** ⁻¹

61: 1474.14 cm**-1
62: 1481.76 cm**-1
63: 1485.84 cm**-1
64: 1492.12 cm**-1
65: 1495.13 cm**-1
66: 1503.90 cm**-1
67: 1505.12 cm**-1
68: 1508.05 cm**-1
69: 1517.17 cm**-1
70: 1549.20 cm**-1
71: 3015.10 cm**-1
72: 3025.28 cm**-1
73: 3030.74 cm**-1
74: 3035.23 cm**-1
75: 3035.77 cm**-1
76: 3043.93 cm**-1
77: 3059.10 cm**-1
78: 3063.48 cm**-1
79: 3071.41 cm**-1
80: 3076.45 cm**-1
81: 3082.09 cm**-1
82: 3088.41 cm**-1
83: 3089.00 cm**-1
84: 3099.36 cm**-1
85: 3106.42 cm**-1
86: 3108.40 cm**-1
87: 3109.73 cm**-1
88: 3118.68 cm**-1
89: 3668.11 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-467.05763638 Eh	
Total entropy correction	...	-0.04967448 Eh	-31.17 kcal/mol

Final Gibbs free energy	...	-467.10731086 Eh	

H₂OH₃O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	-2.864750	0.510500	0.109720
H	-1.895720	0.660550	0.004510
H	-2.820080	-0.184200	0.808040
O	-4.832920	1.365570	-1.160350
H	-5.568650	1.279580	-0.506900
H	-4.001940	0.971290	-0.729460
H	-4.649180	2.314170	-1.360990

FINAL GEOMETRY OPTIMIZATION CYCLE

O	-2.914585	0.354239	0.088100
H	-2.076395	0.238405	-0.384138
H	-2.767565	0.398611	1.044350
O	-4.688444	1.504409	-1.033022
H	-5.502712	1.012170	-1.217173
H	-3.805072	0.964892	-0.434262
H	-4.878468	2.444735	-0.899285

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	192.51	cm** ⁻¹
7:	261.65	cm** ⁻¹
8:	359.66	cm** ⁻¹
9:	485.86	cm** ⁻¹
10:	502.88	cm** ⁻¹
11:	615.15	cm** ⁻¹
12:	951.13	cm** ⁻¹
13:	1461.09	cm** ⁻¹
14:	1521.28	cm** ⁻¹
15:	1679.30	cm** ⁻¹
16:	1765.41	cm** ⁻¹
17:	3741.72	cm** ⁻¹
18:	3750.65	cm** ⁻¹
19:	3832.84	cm** ⁻¹
20:	3834.81	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-153.11310659 Eh	
Total entropy correction	...	-0.03058098 Eh	-19.19 kcal/mol

Final Gibbs free energy	...	-153.14368757	

NH₃H₃O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

N	-1.138030	0.696680	-0.011400
H	-0.123580	0.676570	0.007040
H	-1.463280	0.880440	0.932140
H	-1.463310	-0.226560	-0.278980
O	-0.606550	0.032530	-0.587520
H	0.473890	0.312300	-0.847630
H	-0.876810	-0.705240	-1.253090
H	0.115910	-0.516430	-1.566740

FINAL GEOMETRY OPTIMIZATION CYCLE

N	-1.811290	1.435998	1.147398
H	-1.095895	2.100236	0.942305
H	-1.641522	0.761282	1.873166
H	-2.534265	1.237703	0.477694
O	0.344779	-1.102234	-2.099134
H	0.159343	-0.555542	-1.299326
H	0.542597	-2.040628	-1.908675
H	0.954494	-0.686525	-2.739609

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	25.80	cm** ⁻¹
7:	282.82	cm** ⁻¹
8:	303.18	cm** ⁻¹
9:	325.16	cm** ⁻¹
10:	337.65	cm** ⁻¹
11:	505.54	cm** ⁻¹
12:	1442.74	cm** ⁻¹
13:	1521.96	cm** ⁻¹
14:	1550.60	cm** ⁻¹
15:	1652.76	cm** ⁻¹
16:	1733.55	cm** ⁻¹
17:	1757.85	cm** ⁻¹
18:	2811.93	cm** ⁻¹
19:	3423.90	cm** ⁻¹
20:	3507.61	cm** ⁻¹
21:	3509.22	cm** ⁻¹
22:	3789.89	cm** ⁻¹
23:	3875.78	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-133.26239789 Eh	
Total entropy correction	...	-0.03255709 Eh	-20.43 kcal/mol

Final Gibbs free energy	...	-133.29495498	

C₃H₆OH₃O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	1.261780	5.541500	0.514800
C	1.766090	4.121620	0.688520
H	2.036930	6.250960	0.801700
H	0.372170	5.700210	1.133370
H	0.962970	5.716600	-0.523670
C	0.818630	3.013320	0.271530
H	-0.144900	3.121240	0.779680
H	1.253070	2.041560	0.502740
H	0.620160	3.078990	-0.803580
O	2.867730	3.886420	1.135050
O	3.713950	3.588680	1.552520
H	4.793410	2.939640	1.565460
H	2.560080	2.852140	1.649210
H	3.286860	4.906250	1.434080

FINAL GEOMETRY OPTIMIZATION CYCLE

C	1.542825	5.285589	0.773542
C	1.320985	3.848073	0.489944
H	2.579010	5.524749	1.011462
H	0.915432	5.562181	1.631253
H	1.186808	5.886493	-0.067761
C	0.055223	3.378124	-0.108505
H	-0.787819	3.797978	0.450387
H	-0.003849	2.292586	-0.137205
H	-0.026485	3.790084	-1.121986
O	2.188424	2.968688	0.758371
O	4.367552	3.790587	1.795739
H	5.202218	3.681091	1.315301
H	4.558529	3.651949	2.734198
H	3.070077	3.300958	1.176670

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	93.79	cm** ⁻¹
7:	103.38	cm** ⁻¹
8:	117.90	cm** ⁻¹
9:	126.38	cm** ⁻¹
10:	158.52	cm** ⁻¹
11:	278.93	cm** ⁻¹
12:	391.87	cm** ⁻¹
13:	400.59	cm** ⁻¹
14:	450.13	cm** ⁻¹
15:	499.66	cm** ⁻¹
16:	556.88	cm** ⁻¹
17:	816.24	cm** ⁻¹
18:	880.80	cm** ⁻¹
19:	946.00	cm** ⁻¹
20:	1083.22	cm** ⁻¹
21:	1108.12	cm** ⁻¹
22:	1250.29	cm** ⁻¹
23:	1285.56	cm** ⁻¹
24:	1380.38	cm** ⁻¹
25:	1384.97	cm** ⁻¹
26:	1426.57	cm** ⁻¹
27:	1443.97	cm** ⁻¹

28: 1458.20 cm**⁻¹
29: 1473.48 cm**⁻¹
30: 1494.04 cm**⁻¹
31: 1633.40 cm**⁻¹
32: 1649.61 cm**⁻¹
33: 2668.44 cm**⁻¹
34: 3010.31 cm**⁻¹
35: 3020.67 cm**⁻¹
36: 3082.97 cm**⁻¹
37: 3091.25 cm**⁻¹
38: 3152.15 cm**⁻¹
39: 3157.56 cm**⁻¹
40: 3777.50 cm**⁻¹
41: 3863.13 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-269.76237118 Eh	
Total entropy correction	...	-0.04109214 Eh	-25.79 kcal/mol

Final Gibbs free energy	...	-269.80346332	

C₃H₈OH₃O⁺

CARTESIAN COORDINATES (ANGSTROM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-6.627230	1.426510	-0.445090
C	-5.721920	1.794960	0.722360
H	-6.266740	1.864730	-1.380390
H	-7.640720	1.801210	-0.271030
H	-6.683970	0.340560	-0.572040
C	-4.337290	1.174080	0.597760
H	-6.186130	1.457790	1.655390
H	-5.637020	2.886900	0.764810
O	-3.656610	1.711810	-0.551880
H	-4.401350	0.088750	0.473310
H	-3.733210	1.380840	1.487590
H	-3.236380	2.532100	-0.197580
O	-3.952500	0.939280	-2.900960
H	-3.028680	0.824680	-3.232860
H	-4.412570	0.068990	-2.829100
H	-3.898290	1.335460	-1.972260

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-6.553320	1.344861	-0.570709
C	-5.718844	1.771024	0.636907
H	-6.183421	1.785928	-1.500412
H	-7.583846	1.684538	-0.460505
H	-6.582959	0.254510	-0.669575
C	-4.324950	1.193738	0.686136
H	-6.190200	1.417318	1.562471
H	-5.679471	2.860824	0.730895
O	-3.447307	1.642290	-0.468959
H	-4.287219	0.111990	0.582472
H	-3.753876	1.493227	1.562397
H	-3.169123	2.566766	-0.464103
O	-4.019731	0.997463	-2.698071
H	-3.369023	0.589689	-3.314754
H	-4.887644	0.580870	-2.913513
H	-3.669676	1.333615	-1.352647

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	55.96	cm** ⁻¹
7:	81.92	cm** ⁻¹
8:	129.71	cm** ⁻¹
9:	164.77	cm** ⁻¹
10:	212.58	cm** ⁻¹
11:	231.48	cm** ⁻¹
12:	306.55	cm** ⁻¹
13:	358.00	cm** ⁻¹
14:	408.20	cm** ⁻¹
15:	433.87	cm** ⁻¹
16:	533.70	cm** ⁻¹
17:	741.72	cm** ⁻¹
18:	822.65	cm** ⁻¹
19:	872.51	cm** ⁻¹
20:	900.30	cm** ⁻¹
21:	998.67	cm** ⁻¹
22:	1043.83	cm** ⁻¹
23:	1106.82	cm** ⁻¹

24: 1183.16 cm**⁻¹
 25: 1235.67 cm**⁻¹
 26: 1297.26 cm**⁻¹
 27: 1336.93 cm**⁻¹
 28: 1381.29 cm**⁻¹
 29: 1405.97 cm**⁻¹
 30: 1428.84 cm**⁻¹
 31: 1475.35 cm**⁻¹
 32: 1493.82 cm**⁻¹
 33: 1501.98 cm**⁻¹
 34: 1508.62 cm**⁻¹
 35: 1626.82 cm**⁻¹
 36: 1683.35 cm**⁻¹
 37: 2449.23 cm**⁻¹
 38: 3021.83 cm**⁻¹
 39: 3026.16 cm**⁻¹
 40: 3054.03 cm**⁻¹
 41: 3086.39 cm**⁻¹
 42: 3104.80 cm**⁻¹
 43: 3117.80 cm**⁻¹
 44: 3167.19 cm**⁻¹
 45: 3752.42 cm**⁻¹
 46: 3790.17 cm**⁻¹
 47: 3882.26 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-270.92528541 Eh	
Total entropy correction	...	-0.04185183 Eh	-26.26 kcal/mol

Final Gibbs free energy	...	-270.96713724	

C₄H₆OH₃O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.888100	1.575870	0.019440
C	-4.641300	0.813400	0.145310
C	-3.455800	1.382770	-0.109220
C	-2.126190	0.709700	-0.020910
H	-2.216250	-0.332710	0.290000
H	-1.476710	1.231960	0.690560
H	-1.614200	0.742420	-0.989290
H	-4.728750	-0.226070	0.449580
H	-3.447360	2.430630	-0.410610
O	-6.995790	1.126070	0.222900
H	-5.755540	2.636800	-0.287760
O	-8.151920	0.485380	0.027060
H	-6.818660	0.085020	0.328350
H	-7.597090	1.866680	-0.659220
H	-9.294610	-0.176830	0.296010

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.652486	1.665956	-0.014333
C	-4.535192	0.882270	0.144901
C	-3.291238	1.419596	-0.140745
C	-2.020909	0.702781	-0.031344
H	-2.130998	-0.325324	0.312104
H	-1.353010	1.249747	0.650856
H	-1.511530	0.711607	-1.006589
H	-4.630611	-0.146193	0.485404
H	-3.246115	2.455306	-0.476549
O	-6.899626	1.210529	0.245946
H	-5.620655	2.697062	-0.345694
O	-8.766326	0.324659	-0.015089
H	-6.960560	0.244060	0.446701
H	-7.972858	1.344635	-0.189373
H	-9.616157	-0.085600	-0.073996

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	72.87	cm** ⁻¹
7:	111.49	cm** ⁻¹
8:	140.16	cm** ⁻¹
9:	167.84	cm** ⁻¹
10:	196.43	cm** ⁻¹
11:	210.52	cm** ⁻¹
12:	309.42	cm** ⁻¹
13:	341.39	cm** ⁻¹
14:	403.39	cm** ⁻¹
15:	463.08	cm** ⁻¹
16:	469.02	cm** ⁻¹
17:	553.06	cm** ⁻¹
18:	823.11	cm** ⁻¹
19:	938.74	cm** ⁻¹
20:	982.74	cm** ⁻¹
21:	1017.99	cm** ⁻¹
22:	1074.38	cm** ⁻¹
23:	1144.28	cm** ⁻¹
24:	1224.87	cm** ⁻¹
25:	1247.80	cm** ⁻¹

26: 1299.86 cm**-1
27: 1317.28 cm**-1
28: 1373.35 cm**-1
29: 1385.03 cm**-1
30: 1451.35 cm**-1
31: 1467.93 cm**-1
32: 1472.15 cm**-1
33: 1601.39 cm**-1
34: 1644.35 cm**-1
35: 1652.03 cm**-1
36: 2816.66 cm**-1
37: 3009.07 cm**-1
38: 3046.67 cm**-1
39: 3126.62 cm**-1
40: 3143.62 cm**-1
41: 3148.02 cm**-1
42: 3177.73 cm**-1
43: 3780.03 cm**-1
44: 3866.53 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-307.83036003 Eh	
Total entropy correction	...	-0.04255594 Eh	-26.70 kcal/mol

Final Gibbs free energy	...	-307.87291597	

C₇H₁₂OH₃⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-4.327620	0.493460	0.086280
C	-3.023300	-0.179870	0.221070
C	-1.979400	0.274510	-0.485180
C	-0.608640	-0.343070	-0.444800
C	0.439750	0.696770	-0.048350
H	-0.379990	-0.742120	-1.440330
H	-0.579370	-1.187190	0.254890
C	1.849800	0.109400	-0.072560
H	0.217770	1.080040	0.955720
H	0.391810	1.552130	-0.734580
C	2.885910	1.153470	0.312170
H	2.077840	-0.271370	-1.074980
H	1.914380	-0.737650	0.620000
H	2.862150	2.002010	-0.379310
H	3.890430	0.720510	0.284620
H	2.704650	1.530450	1.323820
H	-2.960040	-1.038440	0.878770
H	-2.089070	1.124220	-1.158240
O	-5.376380	-0.065390	0.415100
H	-4.316480	1.499880	-0.367620
O	-6.246210	-0.951280	0.012290
H	-6.040170	-1.835450	0.400870
H	-6.951720	-0.492870	0.529240
H	-5.407460	-0.392780	0.085310

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-4.254964	0.938718	-0.629860
C	-3.120862	0.127208	-0.451194
C	-1.938605	0.529994	-1.003953
C	-0.649416	-0.167442	-0.882900
C	0.354115	0.689358	-0.052014
H	-0.225237	-0.292870	-1.887719
H	-0.769892	-1.155416	-0.433161
C	1.732374	0.022470	0.028770
H	-0.050669	0.834989	0.954788
H	0.448329	1.681899	-0.505723
C	2.720074	0.845360	0.858774
H	2.123906	-0.117269	-0.984919
H	1.626125	-0.977908	0.462942
H	2.876939	1.836672	0.423796
H	3.691282	0.347824	0.908387
H	2.363846	0.980160	1.884274
H	-3.201614	-0.796938	0.111949
H	-1.929499	1.470219	-1.555777
O	-5.428661	0.705881	-0.187817
H	-4.177840	1.867486	-1.194296
O	-5.670085	-1.498828	1.132823
H	-5.862373	-1.486045	2.079334
H	-6.179905	-2.228900	0.758330
H	-5.528727	-0.157253	0.339366

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	27.97	cm** ⁻¹
7:	57.34	cm** ⁻¹

8:	65.70	cm** ⁻¹
9:	80.30	cm** ⁻¹
10:	118.02	cm** ⁻¹
11:	150.55	cm** ⁻¹
12:	172.21	cm** ⁻¹
13:	184.50	cm** ⁻¹
14:	216.20	cm** ⁻¹
15:	241.44	cm** ⁻¹
16:	279.50	cm** ⁻¹
17:	302.77	cm** ⁻¹
18:	342.36	cm** ⁻¹
19:	395.58	cm** ⁻¹
20:	425.06	cm** ⁻¹
21:	477.17	cm** ⁻¹
22:	505.56	cm** ⁻¹
23:	572.80	cm** ⁻¹
24:	741.51	cm** ⁻¹
25:	805.43	cm** ⁻¹
26:	862.55	cm** ⁻¹
27:	908.35	cm** ⁻¹
28:	936.87	cm** ⁻¹
29:	970.72	cm** ⁻¹
30:	985.52	cm** ⁻¹
31:	1027.66	cm** ⁻¹
32:	1041.66	cm** ⁻¹
33:	1058.56	cm** ⁻¹
34:	1103.61	cm** ⁻¹
35:	1165.39	cm** ⁻¹
36:	1218.88	cm** ⁻¹
37:	1226.51	cm** ⁻¹
38:	1228.35	cm** ⁻¹
39:	1253.23	cm** ⁻¹
40:	1288.88	cm** ⁻¹
41:	1309.01	cm** ⁻¹
42:	1323.48	cm** ⁻¹
43:	1331.11	cm** ⁻¹
44:	1343.78	cm** ⁻¹
45:	1372.56	cm** ⁻¹
46:	1382.05	cm** ⁻¹
47:	1419.52	cm** ⁻¹
48:	1469.37	cm** ⁻¹
49:	1479.79	cm** ⁻¹
50:	1488.29	cm** ⁻¹
51:	1496.19	cm** ⁻¹
52:	1498.70	cm** ⁻¹
53:	1509.69	cm** ⁻¹
54:	1593.19	cm** ⁻¹
55:	1633.03	cm** ⁻¹
56:	1649.02	cm** ⁻¹
57:	2879.43	cm** ⁻¹
58:	3010.41	cm** ⁻¹
59:	3016.63	cm** ⁻¹
60:	3025.48	cm** ⁻¹
61:	3029.94	cm** ⁻¹
62:	3042.50	cm** ⁻¹
63:	3066.99	cm** ⁻¹
64:	3089.35	cm** ⁻¹
65:	3093.56	cm** ⁻¹
66:	3100.22	cm** ⁻¹
67:	3128.88	cm** ⁻¹
68:	3151.00	cm** ⁻¹
69:	3177.26	cm** ⁻¹
70:	3782.36	cm** ⁻¹
71:	3869.57	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-425.64218463 Eh	
Total entropy correction	...	-0.05205267 Eh	-32.66 kcal/mol

Final Gibbs free energy ... -425.69423730

C₇H₁₄OH₃⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.563830	0.681580	-0.081330
C	-4.260150	1.424070	0.072100
H	-5.650120	0.308930	-1.104800
H	-6.398060	1.357020	0.127360
H	-5.601950	-0.149150	0.627500
C	-2.999610	0.576010	0.031670
C	-1.721450	1.410870	0.060260
H	-3.029070	-0.022530	-0.885710
H	-3.024260	-0.102450	0.891590
C	-0.480920	0.517240	0.005240
H	-1.697390	2.022320	0.970820
H	-1.715890	2.106860	-0.787780
C	0.806850	1.340130	0.008470
H	-0.515250	-0.103350	-0.898630
H	-0.483010	-0.164640	0.864460
C	2.036530	0.445920	-0.028800
H	0.846380	1.968900	0.905410
H	0.822840	2.009870	-0.859200
H	2.069060	-0.212550	0.845210
H	2.947440	1.052610	-0.030780
H	2.041640	-0.177570	-0.928650
O	-4.242420	2.655790	0.200280
O	-4.386330	5.104660	0.090350
H	-3.446540	5.344510	0.276930
H	-4.416490	4.097230	0.014390
H	-4.969960	5.362620	0.844050

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.330807	1.312654	-0.214591
C	-3.959840	1.805607	0.066394
H	-5.436410	1.256293	-1.307408
H	-6.104442	1.977511	0.169215
H	-5.461330	0.297703	0.164213
C	-2.806601	0.883305	0.081826
C	-1.411071	1.509903	0.068892
H	-2.950087	0.165878	-0.738172
H	-2.954878	0.267849	0.987276
C	-0.313734	0.440726	0.041860
H	-1.288535	2.150393	0.946969
H	-1.315838	2.159833	-0.807245
C	1.095861	1.040754	0.026067
H	-0.446399	-0.196152	-0.841921
H	-0.419403	-0.216438	0.914416
C	2.192229	-0.025375	-0.024861
H	1.230902	1.666593	0.916106
H	1.192910	1.709205	-0.837729
H	2.140473	-0.690450	0.842486
H	3.184376	0.431407	-0.033117
H	2.103677	-0.642223	-0.924271
O	-3.733458	3.032373	0.284670
O	-5.753200	4.601160	0.353376
H	-5.959541	5.203740	-0.372816
H	-4.550698	3.649018	0.296946
H	-5.976115	5.063630	1.171829

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹

3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 41.90 cm**-1
7: 46.59 cm**-1
8: 62.47 cm**-1
9: 91.69 cm**-1
10: 108.55 cm**-1
11: 125.36 cm**-1
12: 133.72 cm**-1
13: 137.12 cm**-1
14: 157.73 cm**-1
15: 194.13 cm**-1
16: 243.81 cm**-1
17: 285.11 cm**-1
18: 308.14 cm**-1
19: 380.72 cm**-1
20: 410.20 cm**-1
21: 432.41 cm**-1
22: 468.02 cm**-1
23: 488.86 cm**-1
24: 610.97 cm**-1
25: 708.37 cm**-1
26: 743.77 cm**-1
27: 813.05 cm**-1
28: 854.55 cm**-1
29: 913.49 cm**-1
30: 934.62 cm**-1
31: 979.89 cm**-1
32: 1003.93 cm**-1
33: 1028.90 cm**-1
34: 1051.40 cm**-1
35: 1065.22 cm**-1
36: 1130.42 cm**-1
37: 1141.60 cm**-1
38: 1186.66 cm**-1
39: 1224.00 cm**-1
40: 1261.14 cm**-1
41: 1277.64 cm**-1
42: 1286.76 cm**-1
43: 1329.20 cm**-1
44: 1338.62 cm**-1
45: 1344.03 cm**-1
46: 1385.82 cm**-1
47: 1391.74 cm**-1
48: 1397.29 cm**-1
49: 1405.96 cm**-1
50: 1420.61 cm**-1
51: 1437.31 cm**-1
52: 1478.92 cm**-1
53: 1486.58 cm**-1
54: 1489.30 cm**-1
55: 1495.30 cm**-1
56: 1501.22 cm**-1
57: 1501.46 cm**-1
58: 1511.94 cm**-1
59: 1613.90 cm**-1
60: 1649.15 cm**-1
61: 2764.87 cm**-1
62: 2966.07 cm**-1
63: 2998.57 cm**-1
64: 3010.99 cm**-1
65: 3014.69 cm**-1
66: 3020.93 cm**-1
67: 3022.76 cm**-1
68: 3024.75 cm**-1

69: 3035.49 cm**⁻¹
70: 3045.54 cm**⁻¹
71: 3078.72 cm**⁻¹
72: 3085.66 cm**⁻¹
73: 3095.63 cm**⁻¹
74: 3098.54 cm**⁻¹
75: 3149.56 cm**⁻¹
76: 3780.91 cm**⁻¹
77: 3867.61 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-426.84540251 Eh	
Total entropy correction	...	-0.05372113 Eh	-33.71 kcal/mol

Final Gibbs free energy	...	-426.89912364	

C₇H₁₄OH₃⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	3.521720	0.838970	0.083590
C	-0.554000	-0.674530	-0.016230
C	-1.706090	0.330670	0.012800
C	0.808960	0.017640	0.013450
C	-3.056020	-0.387080	-0.020750
C	1.937860	-1.008260	-0.017210
C	-4.216970	0.593210	0.009960
C	3.308470	-0.375460	0.009670
H	-0.638310	-1.350910	0.843210
H	-0.630340	-1.291070	-0.920260
H	-1.627010	1.008350	-0.845900
H	-1.637170	0.945520	0.918390
H	0.893040	0.636070	0.915720
H	0.900980	0.696280	-0.843670
H	-3.128130	-1.000010	-0.926870
H	-3.137170	-1.065940	0.836270
H	1.875820	-1.616110	-0.926310
H	1.869650	-1.678070	0.846800
H	-5.168360	0.052410	-0.016210
H	-4.185430	1.266550	-0.852400
H	-4.195680	1.198640	0.921570
H	4.151140	-1.088980	-0.034360
O	3.906960	3.252920	0.177930
H	4.893270	3.278350	0.130200
H	3.599880	3.451540	1.095470
H	3.632670	2.300520	-0.019510

FINAL GEOMETRY OPTIMIZATION CYCLE

O	3.969474	0.589546	0.232477
C	-0.364479	-0.595858	-0.045979
C	-1.492711	0.433729	0.056961
C	1.025616	0.039251	0.087692
C	-2.887219	-0.185294	-0.084783
C	2.136131	-1.007509	0.021597
C	-4.009434	0.848830	0.027003
C	3.531374	-0.577909	0.141555
H	-0.492259	-1.358216	0.731997
H	-0.431231	-1.118990	-1.007422
H	-1.357992	1.201086	-0.716714
H	-1.424579	0.951346	1.022971
H	1.085607	0.568975	1.046345
H	1.162561	0.777549	-0.708882
H	-2.955847	-0.700405	-1.050137
H	-3.018524	-0.955736	0.684175
H	2.105696	-1.588475	-0.918525
H	2.013228	-1.795699	0.784194
H	-4.989952	0.378613	-0.075713
H	-3.924867	1.611858	-0.753013
H	-3.985436	1.356978	0.995932
H	4.315930	-1.339624	0.156835
O	2.758162	2.766376	0.081310
H	3.343783	3.517675	-0.079868
H	1.975488	3.094916	0.539970
H	3.331220	1.418206	0.205373

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm**-1
1:	0.00	cm**-1
2:	0.00	cm**-1
3:	0.00	cm**-1

4: 0.00 cm**-1
5: 0.00 cm**-1
6: 44.85 cm**-1
7: 55.64 cm**-1
8: 58.73 cm**-1
9: 83.77 cm**-1
10: 102.51 cm**-1
11: 123.86 cm**-1
12: 138.86 cm**-1
13: 149.73 cm**-1
14: 190.61 cm**-1
15: 241.11 cm**-1
16: 245.46 cm**-1
17: 269.88 cm**-1
18: 286.47 cm**-1
19: 336.61 cm**-1
20: 382.25 cm**-1
21: 447.44 cm**-1
22: 478.56 cm**-1
23: 635.85 cm**-1
24: 707.02 cm**-1
25: 738.54 cm**-1
26: 769.38 cm**-1
27: 848.65 cm**-1
28: 889.86 cm**-1
29: 921.82 cm**-1
30: 939.78 cm**-1
31: 1012.35 cm**-1
32: 1018.32 cm**-1
33: 1048.51 cm**-1
34: 1064.91 cm**-1
35: 1072.52 cm**-1
36: 1139.95 cm**-1
37: 1154.69 cm**-1
38: 1209.46 cm**-1
39: 1229.75 cm**-1
40: 1263.17 cm**-1
41: 1274.59 cm**-1
42: 1316.22 cm**-1
43: 1323.06 cm**-1
44: 1337.21 cm**-1
45: 1342.60 cm**-1
46: 1362.85 cm**-1
47: 1374.23 cm**-1
48: 1381.95 cm**-1
49: 1402.08 cm**-1
50: 1417.91 cm**-1
51: 1419.65 cm**-1
52: 1425.44 cm**-1
53: 1486.85 cm**-1
54: 1488.32 cm**-1
55: 1496.76 cm**-1
56: 1501.33 cm**-1
57: 1507.05 cm**-1
58: 1514.38 cm**-1
59: 1639.14 cm**-1
60: 1662.39 cm**-1
61: 2462.92 cm**-1
62: 2962.27 cm**-1
63: 2980.11 cm**-1
64: 2991.29 cm**-1
65: 3005.53 cm**-1
66: 3011.50 cm**-1
67: 3014.13 cm**-1
68: 3017.41 cm**-1
69: 3023.33 cm**-1

70: 3037.55 cm**⁻¹
71: 3049.59 cm**⁻¹
72: 3069.35 cm**⁻¹
73: 3083.32 cm**⁻¹
74: 3097.83 cm**⁻¹
75: 3114.61 cm**⁻¹
76: 3785.69 cm**⁻¹
77: 3878.31 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-426.82083626 Eh	
Total entropy correction	...	-0.05329838 Eh	-33.45 kcal/mol

Final Gibbs free energy	...	-426.87413464	

C₇H₁₂O₂H₃O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.872320	1.914130	-0.419470
C	-4.565910	2.091980	0.304370
H	-6.657570	2.457630	0.103680
H	-6.121590	0.851790	-0.489410
H	-5.780620	2.273470	-1.448560
C	-3.336770	1.355890	-0.300090
C	-2.021590	1.549790	0.409070
C	-0.863560	0.770480	-0.206960
H	-2.170130	1.290220	1.464670
H	-1.816290	2.628370	0.427290
C	0.460140	1.007740	0.525450
H	-0.758720	1.047730	-1.261320
H	-1.102690	-0.298550	-0.203050
C	1.624460	0.225090	-0.086420
H	0.347390	0.731480	1.581130
H	0.693650	2.079630	0.515320
H	1.433490	-0.852360	-0.057220
H	2.558070	0.412490	0.451100
H	1.780200	0.504450	-1.133250
O	-4.428200	2.759960	1.304320
O	-3.487890	0.677910	-1.292060
O	-3.148650	0.089120	-1.942830
H	-2.551350	0.677610	-0.939040
H	-4.379460	0.418700	-1.924250
H	-2.185660	-0.734910	-2.723560

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.011801	2.307601	0.386662
C	-4.574894	1.350918	-0.673158
H	-6.051774	2.581564	0.218261
H	-4.387040	3.205763	0.390635
H	-4.913103	1.842879	1.374502
C	-3.091089	0.853159	-0.682946
C	-2.018479	1.563953	0.033031
C	-0.614898	0.967710	-0.068612
H	-2.348259	1.662885	1.079843
H	-2.045662	2.604846	-0.333772
C	0.413177	1.797979	0.708753
H	-0.323500	0.903232	-1.121608
H	-0.630978	-0.058482	0.312110
C	1.821428	1.207087	0.620814
H	0.106843	1.864620	1.759572
H	0.418548	2.824103	0.322255
H	1.852953	0.195133	1.034807
H	2.534829	1.816498	1.179094
H	2.166512	1.157044	-0.415963
O	-5.276652	0.908049	-1.548235
O	-2.827792	-0.161604	-1.356003
O	-4.474224	-1.506448	-2.570265
H	-4.189795	-2.197217	-3.182092
H	-3.617327	-0.686675	-1.897779
H	-5.268595	-1.074758	-2.910993

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹

6: 32.63 cm**-1
7: 52.34 cm**-1
8: 61.07 cm**-1
9: 81.63 cm**-1
10: 118.34 cm**-1
11: 135.09 cm**-1
12: 139.32 cm**-1
13: 153.29 cm**-1
14: 213.13 cm**-1
15: 230.59 cm**-1
16: 243.22 cm**-1
17: 259.56 cm**-1
18: 309.73 cm**-1
19: 339.56 cm**-1
20: 355.16 cm**-1
21: 400.21 cm**-1
22: 424.79 cm**-1
23: 484.42 cm**-1
24: 539.25 cm**-1
25: 571.11 cm**-1
26: 634.64 cm**-1
27: 730.28 cm**-1
28: 773.18 cm**-1
29: 785.43 cm**-1
30: 913.21 cm**-1
31: 916.65 cm**-1
32: 977.66 cm**-1
33: 1009.63 cm**-1
34: 1029.40 cm**-1
35: 1059.94 cm**-1
36: 1086.46 cm**-1
37: 1106.84 cm**-1
38: 1137.76 cm**-1
39: 1199.07 cm**-1
40: 1217.57 cm**-1
41: 1255.60 cm**-1
42: 1300.37 cm**-1
43: 1301.50 cm**-1
44: 1336.83 cm**-1
45: 1370.70 cm**-1
46: 1380.76 cm**-1
47: 1396.03 cm**-1
48: 1401.24 cm**-1
49: 1413.22 cm**-1
50: 1423.80 cm**-1
51: 1456.16 cm**-1
52: 1461.62 cm**-1
53: 1487.80 cm**-1
54: 1493.81 cm**-1
55: 1501.32 cm**-1
56: 1509.46 cm**-1
57: 1611.35 cm**-1
58: 1665.25 cm**-1
59: 1792.07 cm**-1
60: 1908.33 cm**-1
61: 2969.58 cm**-1
62: 2992.98 cm**-1
63: 3008.58 cm**-1
64: 3028.67 cm**-1
65: 3029.48 cm**-1
66: 3034.76 cm**-1
67: 3036.39 cm**-1
68: 3075.24 cm**-1
69: 3086.95 cm**-1
70: 3091.25 cm**-1
71: 3105.70 cm**-1

72: 3153.87 cm**⁻¹
73: 3777.17 cm**⁻¹
74: 3875.80 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-500.85963123 Eh	
Total entropy correction	...	-0.05430866 Eh	-34.08 kcal/mol

Final Gibbs free energy	...	-500.91393989	

C₁₀H₁₈OH₃O⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	0.123330	-2.123260	0.291570
C	-0.628410	0.163410	0.593410
C	0.232940	1.386940	0.951330
C	2.077540	0.712590	-0.665840
C	1.149730	1.836150	-0.186860
C	-1.801930	0.448940	-0.382890
C	1.270050	-0.521410	-1.055550
C	0.281090	-0.922350	0.018810
C	3.150870	0.366520	0.371690
C	-2.664080	-0.806000	-0.591720
C	-2.710910	1.583390	0.103010
H	-1.041930	-0.223650	1.534730
H	0.849390	1.138630	1.824380
H	-0.388320	2.228710	1.272710
H	2.604480	1.066650	-1.561280
H	0.540320	2.184710	-1.029820
H	1.745710	2.696100	0.140980
H	-1.403530	0.737140	-1.363370
H	1.936590	-1.369270	-1.252140
H	0.701400	-0.334300	-1.973130
H	3.739060	1.253560	0.628880
H	2.723980	-0.036720	1.295060
H	3.841260	-0.385340	-0.026140
H	-3.049390	-1.184560	0.361350
H	-3.520400	-0.588720	-1.239290
H	-2.095970	-1.607400	-1.073620
H	-3.068730	1.396880	1.121200
H	-3.586680	1.687120	-0.547420
H	-2.193160	2.546700	0.088240
O	0.003240	-4.510730	-0.142110
H	0.955460	-4.680250	-0.342790
H	-0.041880	-3.595830	0.286430
H	-0.519860	-4.452110	-0.977990

FINAL GEOMETRY OPTIMIZATION CYCLE

O	-0.170055	-2.027233	0.644075
C	-0.823565	0.233177	0.582800
C	0.200254	1.348009	0.970574
C	1.954452	0.396206	-0.621179
C	1.203461	1.650324	-0.145821
C	-1.899351	0.692761	-0.465700
C	0.911521	-0.696443	-1.050906
C	-0.041946	-0.905402	0.058315
C	2.936596	-0.161747	0.414205
C	-2.715936	-0.502687	-0.974088
C	-2.820974	1.746133	0.156688
H	-1.353496	-0.109739	1.475456
H	0.723572	1.033447	1.877336
H	-0.360578	2.242838	1.241429
H	2.514182	0.642139	-1.527307
H	0.692267	2.110993	-0.996549
H	1.927066	2.388563	0.210438
H	-1.376652	1.146182	-1.314435
H	1.401727	-1.625664	-1.343742
H	0.347864	-0.308108	-1.905609
H	3.687901	0.589951	0.666193
H	2.445431	-0.455912	1.347353
H	3.464109	-1.035899	0.023140
H	-3.209984	-1.023489	-0.148125
H	-3.491820	-0.165316	-1.664138
H	-2.105437	-1.234443	-1.514862
H	-3.348069	1.340562	1.025548

H	-3.573056	2.051795	-0.574527
H	-2.287794	2.645655	0.468035
O	1.236935	-4.003531	-0.258182
H	0.819708	-4.728160	-0.741197
H	0.393119	-2.784927	0.269957
H	1.929809	-4.397796	0.286646

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	36.38	cm** ⁻¹
7:	57.16	cm** ⁻¹
8:	76.79	cm** ⁻¹
9:	88.91	cm** ⁻¹
10:	112.20	cm** ⁻¹
11:	134.07	cm** ⁻¹
12:	150.66	cm** ⁻¹
13:	182.97	cm** ⁻¹
14:	215.04	cm** ⁻¹
15:	222.93	cm** ⁻¹
16:	243.00	cm** ⁻¹
17:	252.39	cm** ⁻¹
18:	307.86	cm** ⁻¹
19:	339.60	cm** ⁻¹
20:	362.77	cm** ⁻¹
21:	369.59	cm** ⁻¹
22:	373.29	cm** ⁻¹
23:	393.45	cm** ⁻¹
24:	418.12	cm** ⁻¹
25:	433.06	cm** ⁻¹
26:	457.79	cm** ⁻¹
27:	525.43	cm** ⁻¹
28:	546.42	cm** ⁻¹
29:	592.76	cm** ⁻¹
30:	711.09	cm** ⁻¹
31:	757.96	cm** ⁻¹
32:	806.98	cm** ⁻¹
33:	831.78	cm** ⁻¹
34:	858.48	cm** ⁻¹
35:	896.75	cm** ⁻¹
36:	913.72	cm** ⁻¹
37:	936.04	cm** ⁻¹
38:	942.99	cm** ⁻¹
39:	959.64	cm** ⁻¹
40:	967.08	cm** ⁻¹
41:	994.81	cm** ⁻¹
42:	1015.73	cm** ⁻¹
43:	1053.49	cm** ⁻¹
44:	1073.74	cm** ⁻¹
45:	1100.12	cm** ⁻¹
46:	1130.64	cm** ⁻¹
47:	1144.93	cm** ⁻¹
48:	1156.02	cm** ⁻¹
49:	1183.06	cm** ⁻¹
50:	1191.07	cm** ⁻¹
51:	1223.35	cm** ⁻¹
52:	1243.97	cm** ⁻¹
53:	1260.27	cm** ⁻¹
54:	1268.08	cm** ⁻¹
55:	1299.49	cm** ⁻¹

56: 1326.71 cm**-1
57: 1349.63 cm**-1
58: 1356.82 cm**-1
59: 1362.35 cm**-1
60: 1366.52 cm**-1
61: 1368.03 cm**-1
62: 1396.29 cm**-1
63: 1412.59 cm**-1
64: 1425.50 cm**-1
65: 1433.16 cm**-1
66: 1475.42 cm**-1
67: 1481.55 cm**-1
68: 1484.62 cm**-1
69: 1488.38 cm**-1
70: 1493.39 cm**-1
71: 1497.74 cm**-1
72: 1505.21 cm**-1
73: 1505.62 cm**-1
74: 1508.82 cm**-1
75: 1517.82 cm**-1
76: 1594.66 cm**-1
77: 1646.83 cm**-1
78: 2898.57 cm**-1
79: 3016.02 cm**-1
80: 3024.01 cm**-1
81: 3027.98 cm**-1
82: 3033.31 cm**-1
83: 3041.17 cm**-1
84: 3043.24 cm**-1
85: 3054.19 cm**-1
86: 3058.87 cm**-1
87: 3067.67 cm**-1
88: 3075.45 cm**-1
89: 3079.89 cm**-1
90: 3086.94 cm**-1
91: 3097.01 cm**-1
92: 3103.18 cm**-1
93: 3103.73 cm**-1
94: 3106.08 cm**-1
95: 3114.24 cm**-1
96: 3114.76 cm**-1
97: 3785.43 cm**-1
98: 3873.64 cm**-1

GIBBS FREE ENERGY

Total enthalpy	...	-543.48625851 Eh	
Total entropy correction	...	-0.05641629 Eh	-35.40 kcal/mol

Final Gibbs free energy	...	-543.54267480 Eh	

H₂ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	-3.154680	0.628800	0.146560
H	-2.205360	0.584110	-0.094170
H	-3.466500	-0.150090	0.653720
H	-3.738070	0.867390	-0.604360
N	-5.075900	-0.848130	1.590540
H	-4.839120	-1.417670	2.359070
H	-6.419750	-0.647860	1.134000
H	-5.983050	-0.795860	2.900470

FINAL GEOMETRY OPTIMIZATION CYCLE

O	-3.349257	0.488255	0.093363
H	-2.387000	0.461121	0.166292
H	-4.421843	-0.266731	1.065464

H	-3.552866	1.063529	-0.654699
N	-5.120729	-0.759556	1.698491
H	-4.739419	-1.657193	2.007772
H	-5.992954	-0.928954	1.191151
H	-5.318363	-0.179781	2.517997

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	9.49	cm** ⁻¹
7:	283.96	cm** ⁻¹
8:	306.52	cm** ⁻¹
9:	326.56	cm** ⁻¹
10:	339.80	cm** ⁻¹
11:	506.94	cm** ⁻¹
12:	1441.55	cm** ⁻¹
13:	1523.09	cm** ⁻¹
14:	1551.00	cm** ⁻¹
15:	1653.10	cm** ⁻¹
16:	1733.22	cm** ⁻¹
17:	1758.41	cm** ⁻¹
18:	2799.72	cm** ⁻¹
19:	3424.03	cm** ⁻¹
20:	3508.48	cm** ⁻¹
21:	3509.60	cm** ⁻¹
22:	3789.75	cm** ⁻¹
23:	3875.45	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-133.26241765 Eh	
Total entropy correction	...	-0.03300077 Eh	-20.71 kcal/mol

Final Gibbs free energy	...	-133.29541842	

NH₃NH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

N	-0.979750	0.436890	0.050460
H	-0.504510	1.312740	-0.196020
H	-1.172160	0.424210	1.058690
H	-1.863470	0.369660	-0.467410
H	-0.378560	-0.358690	-0.193180
N	-1.694860	0.754790	2.574560
H	-0.674860	0.754790	2.574560
H	-2.034860	1.558940	3.101950
H	-2.034860	-0.104020	3.007270

FINAL GEOMETRY OPTIMIZATION CYCLE

N	-1.013878	0.458790	-0.023932
H	-0.395610	1.209179	-0.337997
H	-1.225795	0.554638	1.098792
H	-1.882589	0.513105	-0.559157
H	-0.564715	-0.435513	-0.230000
N	-1.509773	0.687149	2.605574
H	-0.671216	0.908735	3.141671
H	-2.184909	1.423483	2.809710
H	-1.889405	-0.170255	3.006219

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	24.49	cm** ⁻¹
7:	316.28	cm** ⁻¹
8:	396.22	cm** ⁻¹
9:	396.27	cm** ⁻¹
10:	612.54	cm** ⁻¹
11:	612.64	cm** ⁻¹
12:	1265.96	cm** ⁻¹
13:	1345.51	cm** ⁻¹
14:	1580.93	cm** ⁻¹
15:	1581.18	cm** ⁻¹
16:	1667.18	cm** ⁻¹
17:	1667.23	cm** ⁻¹
18:	1667.84	cm** ⁻¹
19:	1758.37	cm** ⁻¹
20:	1758.43	cm** ⁻¹
21:	3428.73	cm** ⁻¹
22:	3445.71	cm** ⁻¹
23:	3523.67	cm** ⁻¹
24:	3524.23	cm** ⁻¹
25:	3542.79	cm** ⁻¹
26:	3542.98	cm** ⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-113.38630706 Eh	
Total entropy correction	...	-0.03176504 Eh	-19.93 kcal/mol

Final Gibbs free energy	...	-113.41807210	

C₃H₆ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	1.033560	5.947530	0.501940
C	1.349790	4.511870	0.712350
H	1.923140	6.574280	0.614520
H	0.287030	6.278530	1.229880
H	0.634350	6.108770	-0.503910
C	0.423000	3.429150	0.297010
H	-0.617700	3.726190	0.456740
H	0.602670	2.516330	0.872990
H	0.560910	3.200530	-0.763900
O	2.554110	4.153600	1.270890
H	3.100650	4.921040	1.515990
N	2.381670	2.754740	0.255420
H	2.725250	3.102740	1.151450
H	1.531150	2.241650	0.484300
H	2.051000	3.604170	-0.211880

FINAL GEOMETRY OPTIMIZATION CYCLE

C	1.070655	5.893937	0.082014
C	0.587092	4.559760	0.569348
H	2.089521	5.841361	-0.300937
H	1.039264	6.603730	0.916941
H	0.401571	6.290743	-0.685893
C	-0.869471	4.406320	0.877588
H	-1.238476	5.262486	1.448678
H	-1.059447	3.476662	1.410748
H	-1.426132	4.400001	-0.067308
O	1.353786	3.605427	0.718822
H	2.816947	3.131346	0.584350
N	3.727415	2.547316	0.580872
H	3.577254	1.707209	1.143997
H	4.505360	3.077919	0.977148
H	3.965241	2.266903	-0.372579

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	1.07	cm** ⁻¹
7:	61.73	cm** ⁻¹
8:	80.10	cm** ⁻¹
9:	92.44	cm** ⁻¹
10:	121.67	cm** ⁻¹
11:	263.46	cm** ⁻¹
12:	383.24	cm** ⁻¹
13:	395.17	cm** ⁻¹
14:	409.31	cm** ⁻¹
15:	498.63	cm** ⁻¹
16:	557.59	cm** ⁻¹
17:	814.16	cm** ⁻¹
18:	883.41	cm** ⁻¹
19:	916.50	cm** ⁻¹
20:	1090.11	cm** ⁻¹
21:	1116.36	cm** ⁻¹
22:	1270.37	cm** ⁻¹
23:	1393.49	cm** ⁻¹
24:	1399.84	cm** ⁻¹
25:	1413.97	cm** ⁻¹

26: 1448.22 cm**⁻¹
 27: 1454.35 cm**⁻¹
 28: 1468.97 cm**⁻¹
 29: 1480.22 cm**⁻¹
 30: 1532.04 cm**⁻¹
 31: 1552.04 cm**⁻¹
 32: 1705.11 cm**⁻¹
 33: 1729.74 cm**⁻¹
 34: 1736.41 cm**⁻¹
 35: 2514.96 cm**⁻¹
 36: 3026.79 cm**⁻¹
 37: 3033.26 cm**⁻¹
 38: 3086.06 cm**⁻¹
 39: 3092.77 cm**⁻¹
 40: 3136.78 cm**⁻¹
 41: 3153.11 cm**⁻¹
 42: 3432.27 cm**⁻¹
 43: 3520.26 cm**⁻¹
 44: 3526.08 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-249.89592433 Eh	
Total entropy correction	...	-0.04401066 Eh	-27.62 kcal/mol

Final Gibbs free energy	...	-249.93993500	

C₃H₈ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-6.626280	1.351750	-0.622110
C	-5.695940	1.775750	0.520970
H	-6.337060	1.779750	-1.591730
H	-7.636560	1.717890	-0.436150
H	-6.680250	0.264490	-0.722650
C	-4.307160	1.207820	0.427960
H	-6.083680	1.401310	1.476380
H	-5.645210	2.863800	0.617810
O	-3.677490	1.748770	-0.903120
H	-4.265660	0.123280	0.331530
H	-3.608700	1.583710	1.171790
H	-2.804690	1.381980	-1.133280
H	-4.290010	1.672500	-1.659390
N	-3.885720	1.307150	-2.548260
H	-5.273900	1.327240	-3.074350
H	-4.097130	1.250100	-3.995010
H	-2.735530	1.218110	-3.758270

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-6.631068	1.504264	-0.507288
C	-5.639074	1.678686	0.644991
H	-6.355222	2.116321	-1.372505
H	-7.634060	1.814819	-0.210010
H	-6.695829	0.455640	-0.819043
C	-4.239860	1.177274	0.330138
H	-5.986062	1.123702	1.523349
H	-5.592265	2.729835	0.952147
O	-3.636162	1.874574	-0.808772
H	-4.250863	0.125474	0.034794
H	-3.563775	1.280271	1.180791
H	-3.392903	2.773752	-0.558036
H	-3.855835	1.433910	-2.251933
N	-4.007501	1.061389	-3.264458
H	-4.963457	0.715119	-3.367955
H	-3.853748	1.809427	-3.943697
H	-3.353288	0.300941	-3.460394

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	37.06	cm** ⁻¹
7:	45.94	cm** ⁻¹
8:	88.39	cm** ⁻¹
9:	164.27	cm** ⁻¹
10:	236.67	cm** ⁻¹
11:	283.60	cm** ⁻¹
12:	312.29	cm** ⁻¹
13:	347.48	cm** ⁻¹
14:	381.79	cm** ⁻¹
15:	476.93	cm** ⁻¹
16:	489.92	cm** ⁻¹
17:	768.02	cm** ⁻¹
18:	857.57	cm** ⁻¹
19:	903.02	cm** ⁻¹
20:	938.47	cm** ⁻¹
21:	1059.38	cm** ⁻¹

22: 1094.96 cm**-1
 23: 1105.68 cm**-1
 24: 1235.46 cm**-1
 25: 1302.61 cm**-1
 26: 1365.71 cm**-1
 27: 1381.57 cm**-1
 28: 1404.74 cm**-1
 29: 1414.53 cm**-1
 30: 1419.83 cm**-1
 31: 1480.49 cm**-1
 32: 1498.50 cm**-1
 33: 1505.86 cm**-1
 34: 1508.42 cm**-1
 35: 1530.84 cm**-1
 36: 1575.53 cm**-1
 37: 1723.57 cm**-1
 38: 1769.27 cm**-1
 39: 2399.64 cm**-1
 40: 3011.34 cm**-1
 41: 3025.98 cm**-1
 42: 3050.22 cm**-1
 43: 3060.66 cm**-1
 44: 3076.49 cm**-1
 45: 3107.26 cm**-1
 46: 3110.17 cm**-1
 47: 3430.56 cm**-1
 48: 3520.90 cm**-1
 49: 3522.19 cm**-1
 50: 3814.16 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-251.06325928 Eh	
Total entropy correction	...	-0.04212718 Eh	-26.44 kcal/mol

Final Gibbs free energy	...	-251.10538645	

C₄H₆ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.798070	1.534670	0.024140
C	-4.632910	0.773340	0.155210
C	-3.427630	1.369020	-0.107730
C	-2.116910	0.713400	-0.022180
H	-2.167940	-0.330540	0.283280
H	-1.475920	1.276610	0.670810
H	-1.609680	0.795150	-0.994150
H	-4.691130	-0.268570	0.458090
H	-3.431190	2.416810	-0.407370
O	-7.002120	1.127790	0.228960
H	-5.761380	2.579530	-0.277260
H	-7.071880	0.195310	0.502470
N	-7.026540	-0.981210	2.735440
H	-5.850720	-0.945910	3.130430
H	-7.734080	-0.504510	3.878320
H	-7.205320	-0.737610	1.502710

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.526407	1.409174	0.355630
C	-4.205343	0.840658	0.357763
C	-3.224138	1.420116	-0.366288
C	-1.821141	0.949115	-0.461793
H	-1.635185	0.055919	0.135153
H	-1.137708	1.744300	-0.142036
H	-1.568352	0.741198	-1.508109
H	-4.022632	-0.052360	0.948657
H	-3.473653	2.314292	-0.937058
O	-6.503952	0.970727	0.974868
H	-5.670704	2.314388	-0.254021
H	-7.037600	-0.106725	1.902413
N	-7.642472	-0.747054	2.537432
H	-7.326626	-0.691877	3.507295
H	-8.613281	-0.430593	2.487274
H	-7.594226	-1.717998	2.223990

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	18.93	cm** ⁻¹
7:	44.58	cm** ⁻¹
8:	75.16	cm** ⁻¹
9:	146.14	cm** ⁻¹
10:	196.54	cm** ⁻¹
11:	205.71	cm** ⁻¹
12:	300.42	cm** ⁻¹
13:	324.50	cm** ⁻¹
14:	402.09	cm** ⁻¹
15:	405.69	cm** ⁻¹
16:	482.62	cm** ⁻¹
17:	553.84	cm** ⁻¹
18:	809.38	cm** ⁻¹
19:	942.27	cm** ⁻¹
20:	984.52	cm** ⁻¹
21:	1036.92	cm** ⁻¹
22:	1075.32	cm** ⁻¹
23:	1124.19	cm** ⁻¹

24: 1200.64 cm**-1
 25: 1293.42 cm**-1
 26: 1332.98 cm**-1
 27: 1402.57 cm**-1
 28: 1405.78 cm**-1
 29: 1426.72 cm**-1
 30: 1464.68 cm**-1
 31: 1476.86 cm**-1
 32: 1531.23 cm**-1
 33: 1553.95 cm**-1
 34: 1665.71 cm**-1
 35: 1669.87 cm**-1
 36: 1727.19 cm**-1
 37: 1733.93 cm**-1
 38: 2450.20 cm**-1
 39: 3011.06 cm**-1
 40: 3018.99 cm**-1
 41: 3062.38 cm**-1
 42: 3116.95 cm**-1
 43: 3133.95 cm**-1
 44: 3159.58 cm**-1
 45: 3433.85 cm**-1
 46: 3522.70 cm**-1
 47: 3529.55 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-287.96097916 Eh	
Total entropy correction	...	-0.04393237 Eh	-27.57 kcal/mol

Final Gibbs free energy	...	-288.00491153	

C₇H₁₂ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-4.264660	0.367330	0.030780
C	-3.033900	-0.270800	0.169130
C	-2.006630	0.082410	-0.671760
C	-0.646960	-0.455490	-0.624720
C	0.333340	0.655850	-0.106590
H	-0.327920	-0.719260	-1.640330
H	-0.580270	-1.339850	0.011670
C	1.777460	0.139270	-0.077420
H	0.023420	0.965190	0.896240
H	0.261540	1.534800	-0.755010
C	2.748120	1.200380	0.446140
H	2.069030	-0.169810	-1.086940
H	1.829690	-0.755260	0.552510
H	2.744350	2.092460	-0.186400
H	3.768030	0.809490	0.462570
H	2.494210	1.506460	1.465020
H	-2.898270	-1.041890	0.922760
H	-2.199660	0.860960	-1.410030
O	-5.328230	0.136810	0.725750
H	-4.420790	1.142650	-0.716030
H	-5.218680	-0.553480	1.403730
N	-5.391410	-0.898140	2.950260
H	-4.499690	-0.974260	3.091940
H	-6.013460	0.278390	2.976380
H	-6.136770	-2.193580	3.723490

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-4.143915	0.394028	0.259014
C	-2.850778	-0.214589	0.396651
C	-1.849941	0.137848	-0.440203
C	-0.465115	-0.392420	-0.417163
C	0.579458	0.723976	-0.183570
H	-0.261401	-0.852586	-1.393843
H	-0.363436	-1.174867	0.340094
C	2.014300	0.186834	-0.208901
H	0.381742	1.206350	0.780255
H	0.462816	1.497970	-0.951048
C	3.055598	1.283806	0.022438
H	2.198180	-0.300459	-1.173506
H	2.122010	-0.591879	0.555212
H	2.993500	2.058182	-0.747927
H	4.067963	0.873831	-0.000436
H	2.915064	1.766940	0.994136
H	-2.703397	-0.959522	1.173506
H	-2.061859	0.894226	-1.196639
O	-5.141146	0.147508	0.951816
H	-4.251036	1.144957	-0.538616
H	-5.697294	-0.649138	2.100744
N	-6.323311	-1.092615	2.874799
H	-5.824070	-1.149799	3.763561
H	-7.152904	-0.508019	2.996465
H	-6.619136	-2.029930	2.596301

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹

6: 12.24 cm**-1
7: 26.08 cm**-1
8: 39.62 cm**-1
9: 66.05 cm**-1
10: 72.61 cm**-1
11: 108.64 cm**-1
12: 147.25 cm**-1
13: 174.75 cm**-1
14: 211.41 cm**-1
15: 241.32 cm**-1
16: 275.33 cm**-1
17: 301.62 cm**-1
18: 347.99 cm**-1
19: 401.64 cm**-1
20: 414.32 cm**-1
21: 446.98 cm**-1
22: 510.89 cm**-1
23: 581.27 cm**-1
24: 739.70 cm**-1
25: 796.33 cm**-1
26: 848.52 cm**-1
27: 905.44 cm**-1
28: 938.59 cm**-1
29: 985.26 cm**-1
30: 1001.72 cm**-1
31: 1040.26 cm**-1
32: 1050.88 cm**-1
33: 1058.94 cm**-1
34: 1114.97 cm**-1
35: 1146.23 cm**-1
36: 1203.86 cm**-1
37: 1226.05 cm**-1
38: 1261.07 cm**-1
39: 1291.68 cm**-1
40: 1318.95 cm**-1
41: 1328.36 cm**-1
42: 1338.28 cm**-1
43: 1354.60 cm**-1
44: 1388.33 cm**-1
45: 1400.99 cm**-1
46: 1418.93 cm**-1
47: 1429.85 cm**-1
48: 1476.67 cm**-1
49: 1488.30 cm**-1
50: 1496.85 cm**-1
51: 1500.13 cm**-1
52: 1510.37 cm**-1
53: 1533.44 cm**-1
54: 1554.46 cm**-1
55: 1656.57 cm**-1
56: 1659.01 cm**-1
57: 1726.25 cm**-1
58: 1732.83 cm**-1
59: 2393.65 cm**-1
60: 3001.43 cm**-1
61: 3009.07 cm**-1
62: 3012.15 cm**-1
63: 3018.66 cm**-1
64: 3025.17 cm**-1
65: 3032.43 cm**-1
66: 3053.91 cm**-1
67: 3073.84 cm**-1
68: 3086.61 cm**-1
69: 3096.82 cm**-1
70: 3120.09 cm**-1
71: 3157.97 cm**-1

72: 3435.45 cm**⁻¹
73: 3524.57 cm**⁻¹
74: 3532.29 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-405.77117832 Eh	
Total entropy correction	...	-0.05359825 Eh	-33.63 kcal/mol

Final Gibbs free energy	...	-405.82477657	

C₇H₁₄ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.565090	0.986190	-0.168500
C	-4.245290	1.582890	0.119850
H	-5.667000	0.944420	-1.263690
H	-6.396380	1.569920	0.232820
H	-5.611950	-0.044560	0.187920
C	-3.004580	0.796340	0.115070
C	-1.679290	1.561710	0.038600
H	-3.100350	0.029310	-0.665360
H	-3.062600	0.210630	1.053600
C	-0.481750	0.605370	0.041950
H	-1.606360	2.255170	0.880940
H	-1.668200	2.169380	-0.872310
C	0.858680	1.343140	-0.042830
H	-0.565940	-0.092210	-0.800860
H	-0.504140	-0.005900	0.953070
C	2.056540	0.391160	-0.041350
H	0.939800	2.039970	0.799620
H	0.875790	1.955610	-0.952080
H	2.085140	-0.209780	0.872480
H	2.996140	0.944290	-0.103500
H	2.019270	-0.295640	-0.892260
O	-4.131740	2.832900	0.374950
H	-4.979200	3.314890	0.398910
N	-5.585070	4.697360	0.423020
H	-4.565070	4.697360	0.423020
H	-5.925070	5.407570	-0.225370
H	-5.925070	4.903780	1.362270

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-5.557234	0.784371	-0.116097
C	-4.251881	1.495340	0.100263
H	-5.683216	0.618375	-1.192817
H	-6.401106	1.371256	0.247635
H	-5.554497	-0.200409	0.355292
C	-2.993683	0.680982	0.059908
C	-1.685577	1.468807	0.055462
H	-3.062995	0.006724	-0.804584
H	-3.041899	0.006335	0.928629
C	-0.458763	0.552915	0.008813
H	-1.641099	2.103736	0.945882
H	-1.673648	2.145713	-0.805865
C	0.864316	1.324961	0.001306
H	-0.510847	-0.083981	-0.883476
H	-0.476579	-0.126828	0.870362
C	2.088365	0.408074	-0.048965
H	0.916232	1.958723	0.895017
H	0.878957	2.005636	-0.858667
H	2.116804	-0.261499	0.816114
H	3.016033	0.985316	-0.052175
H	2.080847	-0.213341	-0.949682
O	-4.205923	2.713872	0.292712
H	-5.056896	3.961451	0.398587
N	-5.448485	4.974752	0.477256
H	-4.668131	5.632568	0.420765
H	-6.102104	5.171156	-0.282595
H	-5.925770	5.106265	1.370899

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00 cm** ⁻¹
1:	0.00 cm** ⁻¹

2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 18.81 cm**-1
7: 36.23 cm**-1
8: 41.35 cm**-1
9: 54.20 cm**-1
10: 82.63 cm**-1
11: 99.68 cm**-1
12: 103.74 cm**-1
13: 120.38 cm**-1
14: 138.65 cm**-1
15: 193.78 cm**-1
16: 243.84 cm**-1
17: 290.18 cm**-1
18: 302.10 cm**-1
19: 393.18 cm**-1
20: 408.01 cm**-1
21: 436.56 cm**-1
22: 465.33 cm**-1
23: 484.93 cm**-1
24: 612.20 cm**-1
25: 719.32 cm**-1
26: 745.33 cm**-1
27: 818.73 cm**-1
28: 851.09 cm**-1
29: 914.50 cm**-1
30: 933.02 cm**-1
31: 966.74 cm**-1
32: 1008.91 cm**-1
33: 1028.69 cm**-1
34: 1058.55 cm**-1
35: 1066.54 cm**-1
36: 1133.93 cm**-1
37: 1149.47 cm**-1
38: 1196.37 cm**-1
39: 1226.83 cm**-1
40: 1280.27 cm**-1
41: 1291.46 cm**-1
42: 1328.72 cm**-1
43: 1336.73 cm**-1
44: 1350.39 cm**-1
45: 1391.78 cm**-1
46: 1401.05 cm**-1
47: 1404.59 cm**-1
48: 1408.76 cm**-1
49: 1418.96 cm**-1
50: 1430.66 cm**-1
51: 1455.73 cm**-1
52: 1478.12 cm**-1
53: 1486.81 cm**-1
54: 1489.95 cm**-1
55: 1500.67 cm**-1
56: 1500.88 cm**-1
57: 1511.93 cm**-1
58: 1536.78 cm**-1
59: 1556.96 cm**-1
60: 1691.46 cm**-1
61: 1730.05 cm**-1
62: 1735.53 cm**-1
63: 2401.34 cm**-1
64: 2992.80 cm**-1
65: 2997.08 cm**-1
66: 3006.37 cm**-1
67: 3017.36 cm**-1

68: 3021.88 cm**-1
69: 3023.07 cm**-1
70: 3027.28 cm**-1
71: 3030.00 cm**-1
72: 3040.21 cm**-1
73: 3068.65 cm**-1
74: 3083.50 cm**-1
75: 3094.36 cm**-1
76: 3095.43 cm**-1
77: 3134.75 cm**-1
78: 3433.78 cm**-1
79: 3523.12 cm**-1
80: 3529.14 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-406.97662178 Eh	
Total entropy correction	...	-0.05515792 Eh	-34.61 kcal/mol

Final Gibbs free energy	...	-407.03177970	

C₇H₁₄ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	3.818610	0.770450	-0.004410
C	-0.449600	-0.656670	0.049180
C	-1.579180	0.367800	-0.071970
C	0.920430	0.007070	-0.111090
C	-2.949300	-0.294720	0.068230
C	2.053810	-1.005170	0.056160
C	-4.073080	0.723820	-0.038280
C	3.410380	-0.503330	-0.300010
H	-0.506590	-1.152760	1.025720
H	-0.573230	-1.432490	-0.716160
H	-1.514080	0.874560	-1.042560
H	-1.461680	1.136390	0.701760
H	1.019830	0.794680	0.643990
H	0.983420	0.484800	-1.096530
H	-3.076990	-1.054180	-0.711920
H	-3.018870	-0.807290	1.034700
H	1.851830	-1.876660	-0.578640
H	2.073570	-1.369360	1.089980
H	-5.044200	0.228720	0.059960
H	-4.048720	1.235490	-1.005720
H	-3.994800	1.477870	0.751460
H	4.254960	-1.156500	-0.473730
H	3.095730	1.413130	0.178250
N	2.434490	3.183810	0.295960
H	1.749920	3.517120	-0.386070
H	3.312260	3.639210	0.031050
H	2.166240	3.624090	1.178480

FINAL GEOMETRY OPTIMIZATION CYCLE

O	3.709231	0.747972	0.038636
C	-0.470711	-0.670366	0.027853
C	-1.618529	0.341781	-0.005080
C	0.910315	-0.006344	0.025064
C	-3.004877	-0.311137	0.001690
C	2.057295	-1.014019	0.036739
C	-4.144922	0.708471	-0.037701
C	3.433373	-0.445568	0.038973
H	-0.565513	-1.302942	0.918310
H	-0.549882	-1.340770	-0.836138
H	-1.522973	0.970913	-0.900805
H	-1.535876	1.015654	0.859016
H	0.992642	0.646666	0.904105
H	0.998289	0.629008	-0.866221
H	-3.086457	-0.987919	-0.856854
H	-3.102137	-0.937588	0.896044
H	2.006880	-1.697695	-0.824207
H	1.999943	-1.686742	0.906041
H	-5.118477	0.212992	-0.031989
H	-4.093920	1.326562	-0.939654
H	-4.109753	1.377360	0.828144
H	4.267348	-1.166099	0.040666
H	2.981159	2.123059	0.053442
N	2.675159	3.157976	0.080423
H	1.667917	3.238023	-0.068576
H	3.166629	3.678966	-0.649025
H	2.913005	3.561665	0.988894

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00 cm** ⁻¹
1:	0.00 cm** ⁻¹

2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 36.74 cm**-1
7: 41.02 cm**-1
8: 48.52 cm**-1
9: 59.50 cm**-1
10: 91.74 cm**-1
11: 93.80 cm**-1
12: 138.58 cm**-1
13: 146.82 cm**-1
14: 190.56 cm**-1
15: 214.83 cm**-1
16: 244.62 cm**-1
17: 272.57 cm**-1
18: 307.10 cm**-1
19: 374.91 cm**-1
20: 402.10 cm**-1
21: 415.27 cm**-1
22: 454.89 cm**-1
23: 660.18 cm**-1
24: 706.76 cm**-1
25: 737.73 cm**-1
26: 769.56 cm**-1
27: 852.91 cm**-1
28: 890.57 cm**-1
29: 922.61 cm**-1
30: 941.48 cm**-1
31: 1014.02 cm**-1
32: 1022.29 cm**-1
33: 1052.57 cm**-1
34: 1064.23 cm**-1
35: 1071.75 cm**-1
36: 1138.40 cm**-1
37: 1165.65 cm**-1
38: 1222.37 cm**-1
39: 1253.12 cm**-1
40: 1278.26 cm**-1
41: 1313.03 cm**-1
42: 1314.82 cm**-1
43: 1335.29 cm**-1
44: 1337.99 cm**-1
45: 1376.81 cm**-1
46: 1395.71 cm**-1
47: 1400.31 cm**-1
48: 1409.93 cm**-1
49: 1417.05 cm**-1
50: 1418.57 cm**-1
51: 1432.21 cm**-1
52: 1486.25 cm**-1
53: 1487.91 cm**-1
54: 1495.74 cm**-1
55: 1501.29 cm**-1
56: 1505.44 cm**-1
57: 1513.29 cm**-1
58: 1541.83 cm**-1
59: 1544.81 cm**-1
60: 1722.93 cm**-1
61: 1734.14 cm**-1
62: 1739.56 cm**-1
63: 2540.96 cm**-1
64: 2980.57 cm**-1
65: 2986.12 cm**-1
66: 2992.21 cm**-1
67: 3005.53 cm**-1

68: 3006.38 cm**-1
69: 3008.14 cm**-1
70: 3010.63 cm**-1
71: 3016.55 cm**-1
72: 3020.96 cm**-1
73: 3024.19 cm**-1
74: 3041.73 cm**-1
75: 3057.56 cm**-1
76: 3080.22 cm**-1
77: 3095.69 cm**-1
78: 3431.48 cm**-1
79: 3519.81 cm**-1
80: 3527.80 cm**-1

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T \cdot S$

Total enthalpy	...	-406.96084112 Eh	
Total entropy correction	...	-0.05388252 Eh	-33.81 kcal/mol

Final Gibbs free energy	...	-407.01472364	

C₇H₁₂O₂NH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

C	-5.867060	1.924390	-0.419770
C	-4.581880	2.109510	0.316230
H	-6.650590	2.480650	0.091400
H	-6.133390	0.863540	-0.469560
H	-5.772200	2.277810	-1.451940
C	-3.315040	1.391050	-0.230820
C	-2.013830	1.538340	0.416250
C	-0.853320	0.760020	-0.204570
H	-2.173570	1.302330	1.481510
H	-1.824680	2.625110	0.460450
C	0.470340	1.010450	0.536810
H	-0.721840	1.054390	-1.255650
H	-1.069020	-0.316960	-0.181500
C	1.636800	0.239270	-0.080800
H	0.347120	0.725570	1.587270
H	0.684280	2.084700	0.526150
H	1.461600	-0.840040	-0.052240
H	2.560090	0.438280	0.466030
H	1.800190	0.529610	-1.122660
O	-4.396310	2.763910	1.307120
O	-3.494120	0.679300	-1.268840
H	-2.672220	0.243510	-1.583590
N	-3.697370	0.122020	-2.101320
H	-2.677370	0.122020	-2.101320
H	-4.037360	0.528580	-1.229820
H	-4.037370	-0.836000	-2.184980

FINAL GEOMETRY OPTIMIZATION CYCLE

C	-4.910996	2.378317	0.616246
C	-4.525214	1.479769	-0.515204
H	-5.985215	2.553792	0.599719
H	-4.382136	3.334207	0.532196
H	-4.619445	1.941811	1.576261
C	-3.021961	1.036538	-0.686089
C	-2.035607	1.310818	0.399984
C	-0.605491	0.854805	0.115787
H	-2.427223	0.836224	1.313234
H	-2.075147	2.386911	0.622375
C	0.339997	1.161224	1.282327
H	-0.244667	1.343976	-0.794812
H	-0.603106	-0.219738	-0.093094
C	1.774896	0.705769	1.009497
H	-0.033614	0.673140	2.190605
H	0.329335	2.238766	1.485924
H	1.822416	-0.374029	0.839725
H	2.427552	0.937625	1.853989
H	2.186649	1.201853	0.125550
O	-5.309390	1.065510	-1.341882
O	-2.731940	0.459469	-1.721645
H	-4.321808	0.163061	-4.541977
N	-4.479591	-0.305583	-3.648678
H	-5.383123	-0.023898	-3.256763
H	-3.759939	-0.002043	-2.926728
H	-4.453354	-1.316936	-3.786708

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹

4: 0.00 cm**-1
5: 0.00 cm**-1
6: 35.20 cm**-1
7: 49.66 cm**-1
8: 62.78 cm**-1
9: 77.04 cm**-1
10: 98.12 cm**-1
11: 110.33 cm**-1
12: 126.68 cm**-1
13: 142.03 cm**-1
14: 146.18 cm**-1
15: 207.31 cm**-1
16: 232.13 cm**-1
17: 242.74 cm**-1
18: 282.23 cm**-1
19: 316.56 cm**-1
20: 348.32 cm**-1
21: 361.86 cm**-1
22: 386.31 cm**-1
23: 440.88 cm**-1
24: 483.96 cm**-1
25: 578.90 cm**-1
26: 629.35 cm**-1
27: 733.12 cm**-1
28: 785.66 cm**-1
29: 792.20 cm**-1
30: 917.30 cm**-1
31: 919.90 cm**-1
32: 973.02 cm**-1
33: 1012.35 cm**-1
34: 1025.08 cm**-1
35: 1062.74 cm**-1
36: 1078.42 cm**-1
37: 1116.44 cm**-1
38: 1135.63 cm**-1
39: 1205.40 cm**-1
40: 1229.16 cm**-1
41: 1296.87 cm**-1
42: 1306.81 cm**-1
43: 1334.39 cm**-1
44: 1377.42 cm**-1
45: 1391.77 cm**-1
46: 1393.62 cm**-1
47: 1403.69 cm**-1
48: 1417.57 cm**-1
49: 1421.41 cm**-1
50: 1458.38 cm**-1
51: 1462.91 cm**-1
52: 1487.79 cm**-1
53: 1494.72 cm**-1
54: 1501.13 cm**-1
55: 1509.90 cm**-1
56: 1511.50 cm**-1
57: 1572.77 cm**-1
58: 1713.55 cm**-1
59: 1736.60 cm**-1
60: 1739.94 cm**-1
61: 1777.61 cm**-1
62: 2784.35 cm**-1
63: 2988.72 cm**-1
64: 3006.80 cm**-1
65: 3012.69 cm**-1
66: 3025.36 cm**-1
67: 3031.57 cm**-1
68: 3031.98 cm**-1
69: 3033.86 cm**-1

70: 3070.97 cm**⁻¹
71: 3086.96 cm**⁻¹
72: 3087.35 cm**⁻¹
73: 3100.23 cm**⁻¹
74: 3151.29 cm**⁻¹
75: 3420.33 cm**⁻¹
76: 3511.37 cm**⁻¹
77: 3534.48 cm**⁻¹

GIBBS FREE ENERGY

The Gibbs free energy is $G = H - T*S$

Total enthalpy	...	-481.00261178 Eh	
Total entropy correction	...	-0.05554441 Eh	-34.85 kcal/mol

Final Gibbs free energy	...	-481.05815619 Eh	

C₁₀H₁₈ONH₄⁺

CARTESIAN COORDINATES (ANGSTROEM)

INPUT GEOMETRY OPTIMIZATION CYCLE

O	0.071380	-2.141540	0.162330
C	-0.632090	0.139000	0.573020
C	0.236030	1.341130	0.980830
C	2.087100	0.717300	-0.644760
C	1.158090	1.826540	-0.137030
C	-1.799660	0.468240	-0.397340
C	1.281630	-0.503240	-1.079010
C	0.268130	-0.933890	-0.038540
C	3.153870	0.338120	0.387700
C	-2.688380	-0.764150	-0.629590
C	-2.684390	1.612520	0.109190
H	-1.052350	-0.279090	1.497960
H	0.847880	1.055110	1.845490
H	-0.380720	2.173860	1.333020
H	2.620360	1.099190	-1.524980
H	0.553680	2.202080	-0.971980
H	1.752810	2.675090	0.221260
H	-1.395010	0.765670	-1.372600
H	1.949240	-1.347520	-1.287290
H	0.730810	-0.287810	-2.001430
H	3.733420	1.218330	0.685040
H	2.721830	-0.104800	1.290200
H	3.853250	-0.392220	-0.033780
H	-3.076450	-1.156390	0.316830
H	-3.543540	-0.515490	-1.267330
H	-2.139420	-1.565670	-1.132800
H	-3.039040	1.419200	1.127180
H	-3.562030	1.741810	-0.534030
H	-2.147900	2.565730	0.103400
N	-0.213070	-4.413180	-0.921090
H	-1.083350	-4.330190	-1.452350
H	0.595770	-4.409750	-1.547430
H	-0.217980	-5.251350	-0.335210
H	-0.062450	-3.147350	-0.234870

FINAL GEOMETRY OPTIMIZATION CYCLE

O	-0.197194	-2.092469	0.118784
C	-0.826459	0.171976	0.503996
C	0.222294	1.181748	1.049083
C	1.904442	0.538749	-0.762189
C	1.179141	1.686678	-0.036161
C	-1.910599	0.815676	-0.417805
C	0.857278	-0.474496	-1.312560
C	-0.075896	-0.907208	-0.221229
C	2.940412	-0.166936	0.121148
C	-2.798578	-0.260568	-1.056097
C	-2.765714	1.814968	0.369453
H	-1.343634	-0.306020	1.341161
H	0.787755	0.696970	1.850645
H	-0.299993	2.016927	1.517401
H	2.427377	0.952347	-1.629445
H	0.630617	2.287699	-0.768139
H	1.919721	2.354961	0.412027
H	-1.403941	1.363218	-1.220209
H	1.344608	-1.341350	-1.766605
H	0.261154	0.021800	-2.085947
H	3.683430	0.546017	0.485916
H	2.488802	-0.644775	0.996417
H	3.475803	-0.937381	-0.442319
H	-3.291159	-0.866873	-0.289195
H	-3.577791	0.200180	-1.667025

H	-2.235795	-0.938469	-1.706343
H	-3.270757	1.324734	1.207858
H	-3.535918	2.238464	-0.279769
H	-2.181499	2.647810	0.764465
N	0.704897	-4.430930	-0.403367
H	0.383698	-4.801418	-1.298849
H	1.720536	-4.519604	-0.352140
H	0.288899	-4.984604	0.347944
H	0.391514	-3.372531	-0.280893

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.00000000 (already applied!)

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	26.52	cm** ⁻¹
7:	31.98	cm** ⁻¹
8:	46.40	cm** ⁻¹
9:	53.95	cm** ⁻¹
10:	87.28	cm** ⁻¹
11:	113.49	cm** ⁻¹
12:	152.73	cm** ⁻¹
13:	182.14	cm** ⁻¹
14:	216.77	cm** ⁻¹
15:	224.25	cm** ⁻¹
16:	242.39	cm** ⁻¹
17:	255.16	cm** ⁻¹
18:	317.01	cm** ⁻¹
19:	346.54	cm** ⁻¹
20:	366.22	cm** ⁻¹
21:	378.75	cm** ⁻¹
22:	398.17	cm** ⁻¹
23:	427.18	cm** ⁻¹
24:	436.09	cm** ⁻¹
25:	441.11	cm** ⁻¹
26:	478.45	cm** ⁻¹
27:	551.23	cm** ⁻¹
28:	557.27	cm** ⁻¹
29:	593.36	cm** ⁻¹
30:	712.40	cm** ⁻¹
31:	755.16	cm** ⁻¹
32:	813.51	cm** ⁻¹
33:	826.74	cm** ⁻¹
34:	865.84	cm** ⁻¹
35:	900.91	cm** ⁻¹
36:	922.57	cm** ⁻¹
37:	935.68	cm** ⁻¹
38:	952.98	cm** ⁻¹
39:	966.50	cm** ⁻¹
40:	969.73	cm** ⁻¹
41:	995.35	cm** ⁻¹
42:	1019.37	cm** ⁻¹
43:	1056.47	cm** ⁻¹
44:	1074.42	cm** ⁻¹
45:	1099.21	cm** ⁻¹
46:	1134.53	cm** ⁻¹
47:	1152.43	cm** ⁻¹
48:	1166.85	cm** ⁻¹
49:	1185.50	cm** ⁻¹
50:	1212.37	cm** ⁻¹
51:	1248.37	cm** ⁻¹
52:	1278.67	cm** ⁻¹

53: 1287.12 cm**-1
 54: 1301.54 cm**-1
 55: 1326.56 cm**-1
 56: 1353.80 cm**-1
 57: 1358.81 cm**-1
 58: 1366.27 cm**-1
 59: 1368.53 cm**-1
 60: 1379.55 cm**-1
 61: 1382.93 cm**-1
 62: 1397.75 cm**-1
 63: 1409.82 cm**-1
 64: 1420.66 cm**-1
 65: 1430.48 cm**-1
 66: 1473.27 cm**-1
 67: 1484.60 cm**-1
 68: 1487.24 cm**-1
 69: 1494.46 cm**-1
 70: 1499.22 cm**-1
 71: 1505.45 cm**-1
 72: 1505.70 cm**-1
 73: 1508.55 cm**-1
 74: 1519.06 cm**-1
 75: 1549.65 cm**-1
 76: 1562.93 cm**-1
 77: 1657.99 cm**-1
 78: 1728.56 cm**-1
 79: 1731.92 cm**-1
 80: 2106.93 cm**-1
 81: 3017.36 cm**-1
 82: 3018.39 cm**-1
 83: 3020.83 cm**-1
 84: 3028.98 cm**-1
 85: 3031.99 cm**-1
 86: 3034.91 cm**-1
 87: 3042.75 cm**-1
 88: 3048.02 cm**-1
 89: 3056.73 cm**-1
 90: 3073.35 cm**-1
 91: 3074.83 cm**-1
 92: 3078.41 cm**-1
 93: 3080.72 cm**-1
 94: 3091.34 cm**-1
 95: 3094.88 cm**-1
 96: 3097.56 cm**-1
 97: 3100.35 cm**-1
 98: 3109.25 cm**-1
 99: 3436.84 cm**-1
 100: 3528.94 cm**-1
 101: 3536.49 cm**-1

GIBBS FREE ENERGY

Total enthalpy	...	-523.61370268 Eh	
Total entropy correction	...	-0.05703075 Eh	-35.79 kcal/mol

Final Gibbs free energy	...	-523.67073343 Eh	