Supporting Information

A Substantial Oxygen Isotope Effect at O2 in the OMP Decarboxylase Reaction: Mechanistic Implications

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GAS PHASE

6-deprotonated 1-methyl uracil

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -453.556115607

Zero-point correction= 0.100928
(Hartree/Particle)
Thermal correction to Energy= 0.108561
Thermal correction to Enthalpy= 0.109505
Thermal correction to Gibbs Free Energy= 0.068599
Sum of electronic and zero-point Energies= -453.455188
Sum of electronic and thermal Energies= -453.447555
Sum of electronic and thermal Enthalpies= -453.446611
Sum of electronic and thermal Free Energies= -453.487517

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	68.123	28.108	86.093

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.065176	-0.511459	-0.000022
2	6	0	-0.659112	0.811289	-0.000004
3	7	0	0.709010	0.982486	-0.000028

4	6	0	1.694959	-0.031376	-0.000002
5	6	0	1.134015	-1.351884	0.000018
6	6	0	-0.223110	-1.641347	0.000010
7	6	0	-2.513501	-0.710417	-0.000010
8	8	0	-1.438685	1.779855	0.000031
9	1	0	1.036717	1.941104	-0.000007
10	8	0	2.891895	0.316337	0.000000
11	1	0	1.854142	-2.167340	0.000041
12	1	0	-2.673920	-1.788684	-0.000192
13	1	0	-2.974458	-0.254861	0.885886
14	1	0	-2.974509	-0.254532	-0.885704

1-methyl orotate

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.206013214

Zero-point correction= 0.116200
(Hartree/Particle)
Thermal correction to Energy= 0.126895
Thermal correction to Enthalpy= 0.127839
Thermal correction to Gibbs Free Energy= 0.078210
Sum of electronic and zero-point Energies= -642.089813
Sum of electronic and thermal Energies= -642.079118
Sum of electronic and thermal Enthalpies= -642.078174
Sum of electronic and thermal Free Energies= -642.127804

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	79.628	37.673	104.455

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.147660	0.899634	-0.052186
2	6	0	-1.205426	1.216322	-0.036533
3	7	0	-2.048004	0.123626	0.011819
4	6	0	-1.698964	-1.244390	0.042197
5	6	0	-0.280798	-1.461254	0.022875
6	6	0	0.598145	-0.413932	-0.010807
7	6	0	1.111398	2.008551	-0.088449
8	8	0	-1.643823	2.369306	-0.065618
9	1	0	-3.038128	0.339049	0.022843
10	8	0	-2.600376	-2.090368	0.079511
11	1	0	0.087374	-2.479186	0.031198
12	6	0	2.129909	-0.623270	0.025136
13	8	0	2.632921	-1.030153	-1.045018
14	8	0	2.647603	-0.340729	1.131544
15	1	0	1.836522	1.828321	-0.885994
16	1	0	0.556252	2.925620	-0.278935
17	1	0	1.644201	2.066773	0.863597

2-protonated, 6-deprotonated 1-methyl uracil (favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -454.034797905

Zero-point correction= 0.112664
(Hartree/Particle)
Thermal correction to Energy= 0.120824
Thermal correction to Enthalpy= 0.121768
Thermal correction to Gibbs Free Energy= 0.079944
Sum of electronic and zero-point Energies= -453.922134
Sum of electronic and thermal Energies= -453.913974
Sum of electronic and thermal Enthalpies= -453.913030
Sum of electronic and thermal Free Energies= -453.954854

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	75.818	30.400	88.027

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.696674	0.988815	-0.000066
2	6	0	-1.740830	-0.018136	0.000051
3	6	0	-1.194935	-1.349930	-0.000009
4	6	0	0.140053	-1.689499	-0.000036
5	7	0	1.026453	-0.545541	-0.000049
6	6	0	0.604605	0.713738	-0.000045
7	1	0	-0.995507	1.959534	0.000012
8	8	0	-2.898164	0.376998	0.000049
9	1	0	-1.932437	-2.147465	-0.000043
10	8	0	1.414536	1.786198	-0.000014
11	6	0	2.469911	-0.821049	0.000050
12	1	0	2.556367	-1.907163	-0.000454
13	1	0	2.954506	-0.424071	-0.901755
14	1	0	2.954204	-0.424979	0.902405
15	1	0	2.350602	1.524923	0.000292

2-protonated 1-methyl orotate (favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.647673668

Zero-point correction= 0.127866
(Hartree/Particle)
Thermal correction to Energy= 0.138629
Thermal correction to Enthalpy= 0.139573
Thermal correction to Gibbs Free Energy= 0.090610
Sum of electronic and zero-point Energies= -642.519808
Sum of electronic and thermal Energies= -642.509044
Sum of electronic and thermal Enthalpies= -642.508100

Sum of electronic and thermal Free Energies= -642.557064

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.991	39.564	103.053

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.038868	-0.050632	0.046982
2	6	0	-1.560300	-1.417204	0.082816
3	6	0	-0.123840	-1.480973	0.012912
4	6	0	0.669328	-0.376992	-0.029401
5	7	0	0.072438	0.915560	-0.043597
6	6	0	-1.256167	1.021607	-0.037516
7	1	0	-3.047143	0.081552	0.053987
8	8	0	-2.382601	-2.309440	0.152937
9	1	0	0.348716	-2.455073	-0.017981
10	8	0	-1.892375	2.185444	-0.123654
11	6	0	2.233488	-0.522162	0.020283
12	8	0	2.780088	0.295848	0.798005
13	8	0	2.662410	-1.444156	-0.681362
14	6	0	0.887705	2.151953	-0.147781
15	1	0	1.918980	1.859504	0.068258
16	1	0	0.795436	2.579223	-1.151844
17	1	0	0.582956	2.864689	0.626222
18	1	0	-1.275401	2.936667	-0.177613

Decarboxylation pathway for 2-protonated 1-methyl orotate r=1.9 (favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.638974945

Zero-point correction= 0.126398
(Hartree/Particle)
Thermal correction to Energy= 0.136901
Thermal correction to Enthalpy= 0.137845
Thermal correction to Gibbs Free Energy= 0.089411
Sum of electronic and zero-point Energies= -642.512577
Sum of electronic and thermal Energies= -642.502074
Sum of electronic and thermal Enthalpies= -642.501130
Sum of electronic and thermal Free Energies= -642.549564

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.906	38.702	101.938

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	2.098377	-0.184629	-0.000232
2	6	0	1.504294	-1.507113	-0.000022
3	6	0	0.062700	-1.442208	-0.000083
4	6	0	-0.637428	-0.278925	0.000088
5	7	0	0.074772	0.948228	0.000211
6	6	0	1.407984	0.952611	-0.000125
7	1	0	3.114179	-0.139496	-0.000461
8	8	0	2.252341	-2.465849	0.000173
9	1	0	-0.494213	-2.372897	-0.000161
10	8	0	2.135417	2.068111	-0.000226
11	6	0	-2.532136	-0.420626	-0.000158
12	8	0	-3.076005	0.676559	-0.000764
13	8	0	-2.789969	-1.603227	0.000374
14	6	0	-0.647713	2.242190	0.000757
15	1	0	-1.715562	1.999833	0.000789
16	1	0	-0.405821	2.811052	0.905915
17	1	0	-0.406377	2.811576	-0.904256
18	1	0	1.575276	2.864418	-0.000865

Decarboxylation pathway for 2-protonated 1-methyl orotate r=2.0 (favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.635966555

Zero-point correction= 0.126214
(Hartree/Particle)
Thermal correction to Energy= 0.136847
Thermal correction to Enthalpy= 0.137791
Thermal correction to Gibbs Free Energy= 0.089114
Sum of electronic and zero-point Energies= -642.509752
Sum of electronic and thermal Energies= -642.499120
Sum of electronic and thermal Enthalpies= -642.498176
Sum of electronic and thermal Free Energies= -642.546852

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.873	38.979	102.448

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.115925	-0.206992	0.000058
2	6	0	-1.503266	-1.522248	0.000058
3	6	0	-0.062919	-1.436834	0.000058
4	6	0	0.626056	-0.264915	0.000058
5	7	0	-0.108562	0.949160	0.000058
6	6	0	-1.441481	0.939576	0.000058
7	1	0	-3.132151	-0.176608	0.000058
8	8	0	-2.240743	-2.490035	0.000058
9	1	0	0.500296	-2.364059	0.000012

10	8	0	-2.184281	2.046635	0.000058
11	6	0	2.621518	-0.399570	0.000058
12	8	0	3.121741	0.708588	-0.000693
13	8	0	2.850108	-1.581009	0.000157
14	6	0	0.604753	2.246245	0.000058
15	1	0	1.673472	2.015864	0.000188
16	1	0	0.361180	2.816257	-0.904181
17	1	0	0.361042	2.816332	0.904211
18	1	0	-1.635003	2.850077	0.000204

Decarboxylation pathway for 2-protonated 1-methyl orotate r=2.2 (favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.632035651

Zero-point correction= 0.125781
(Hartree/Particle)
Thermal correction to Energy= 0.136713
Thermal correction to Enthalpy= 0.137657
Thermal correction to Gibbs Free Energy= 0.088140
Sum of electronic and zero-point Energies= -642.506255
Sum of electronic and thermal Energies= -642.495322
Sum of electronic and thermal Enthalpies= -642.494378
Sum of electronic and thermal Free Energies= -642.543896

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.789	39.511	104.219

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.151509	-0.248277	0.000068
2	6	0	-1.504658	-1.547864	0.000068
3	6	0	-0.067593	-1.425549	0.000068
4	6	0	0.607988	-0.240614	0.000068
5	7	0	-0.173937	0.950535	0.000068
6	6	0	-1.504976	0.914047	0.000068
7	1	0	-3.167876	-0.244164	0.000068
8	8	0	-2.221250	-2.533214	0.000068
9	1	0	0.504002	-2.348246	0.000133
10	8	0	-2.277851	2.004051	0.000068
11	6	0	2.804712	-0.360634	-0.000178
12	8	0	3.214951	0.766982	-0.000909
13	8	0	2.966957	-1.539927	0.000481
14	6	0	0.515975	2.256258	0.000068
15	1	0	1.585875	2.045273	-0.000184
16	1	0	0.266800	2.827055	-0.902828
17	1	0	0.267145	2.826873	0.903172
18	1	0	-1.748971	2.820391	0.000068

Decarboxylation pathway for 2-protonated 1-methyl orotate r=2.4 (potential energy maximum, favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.630703954

Zero-point correction= 0.125296
(Hartree/Particle)
Thermal correction to Energy= 0.136566
Thermal correction to Enthalpy= 0.137510
Thermal correction to Gibbs Free Energy= 0.086775
Sum of electronic and zero-point Energies= -642.505408
Sum of electronic and thermal Energies= -642.494138
Sum of electronic and thermal Enthalpies= -642.493194
Sum of electronic and thermal Free Energies= -642.543929

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.696	39.993	106.781

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.195223	-0.288035	0.000002
2	6	0	-1.516956	-1.570952	-0.000005
3	6	0	-0.084123	-1.414415	-0.000007
4	6	0	0.584199	-0.218636	-0.000002
5	7	0	-0.245573	0.950889	0.000006
6	6	0	-1.574109	0.888089	0.000007
7	1	0	-3.211111	-0.307658	0.000004
8	8	0	-2.212788	-2.573329	-0.000009
9	1	0	0.494838	-2.333053	-0.000013
10	8	0	-2.375633	1.961085	0.000014
11	6	0	3.026038	-0.323521	-0.000007
12	8	0	3.327729	0.822756	-0.000002
13	8	0	3.105127	-1.499275	-0.000014
14	6	0	0.415900	2.267963	0.000011
15	1	0	1.487849	2.075395	0.000009
16	1	0	0.159418	2.837615	-0.902199
17	1	0	0.159420	2.837606	0.902228
18	1	0	-1.866014	2.789061	0.000018

4-protonated, 6-deprotonated 1-methyl uracil (favored conformer, proton toward C5)

B3lyp/6-31+G*

Done: E(RB+HF-LYP) = -454.061592225

Zero-point correction= 0.113774
(Hartree/Particle)
Thermal correction to Energy= 0.121662

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 Thermal correction to Enthalpy=                 0.122606
 Thermal correction to Gibbs Free Energy=        0.081423
 Sum of electronic and zero-point Energies=           -453.947819
 Sum of electronic and thermal Energies=              -453.939930
 Sum of electronic and thermal Enthalpies=            -453.938986
 Sum of electronic and thermal Free Energies=         -453.980169

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  76.344             29.768            86.676

                         Standard orientation:
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
    1          7             0        0.682499    0.981171    0.000057
    2          6             0        1.560278   -0.057160    0.000013
    3          6             0        1.088536   -1.345262   -0.000115
    4          6             0       -0.305705   -1.630073   -0.000091
    5          7             0       -1.109319   -0.521344   -0.000014
    6          6             0       -0.702808    0.821635   -0.000014
    7          1             0        1.022745    1.936828    0.000083
    8          8             0        2.844630    0.356788    0.000085
    9          1             0        1.795637   -2.171505   -0.000159
   10          8             0       -1.456085    1.782965   -0.000142
   11          6             0       -2.573733   -0.698469    0.000156
   12          1             0       -2.754601   -1.771477    0.000116
   13          1             0       -3.009578   -0.230182    0.887369
   14          1             0       -3.009906   -0.230251   -0.887004
   15          1             0        3.435681   -0.414253    0.000053
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4-protonated 1-methyl orotate (favored conformer, proton toward C5)

B3lyp/6-31+G*

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SCF Done:  E(RB+HF-LYP) =  -642.672852399

Zero-point correction=                          0.128154
(Hartree/Particle)
 Thermal correction to Energy=                   0.139393
 Thermal correction to Enthalpy=                 0.140337
 Thermal correction to Gibbs Free Energy=        0.088829
 Sum of electronic and zero-point Energies=           -642.544699
 Sum of electronic and thermal Energies=              -642.533460
 Sum of electronic and thermal Enthalpies=            -642.532516
 Sum of electronic and thermal Free Energies=         -642.584023

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  87.470             39.657           108.406

                         Standard orientation:
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	7	0	2.013170	0.237167	-0.000900
2	6	0	1.653506	-1.073363	0.003799
3	6	0	0.323999	-1.413914	0.002345
4	6	0	-0.626499	-0.381223	-0.003625
5	7	0	-0.233119	0.919015	-0.012416
6	6	0	1.115295	1.309653	-0.005026
7	1	0	2.996554	0.489989	0.003381
8	8	0	2.703444	-1.901817	0.009344
9	1	0	-0.006496	-2.445654	0.004736
10	8	0	1.505392	2.459801	-0.003558
11	6	0	-1.253442	1.992903	-0.012106
12	1	0	-0.739811	2.946114	-0.113046
13	1	0	-1.932632	1.824896	-0.849684
14	1	0	-1.810323	1.949327	0.926204
15	1	0	2.411613	-2.829394	0.013434
16	6	0	-2.129266	-0.702540	0.003909
17	8	0	-2.597286	-0.846406	-1.138862
18	8	0	-2.596652	-0.763785	1.154626

Decarboxylation pathway for 4-protonated 1-methyl orotate r=1.9 (favored conformer, proton toward C5)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.662469073

Zero-point correction= 0.127189
(Hartree/Particle)
Thermal correction to Energy= 0.137669
Thermal correction to Enthalpy= 0.138613
Thermal correction to Gibbs Free Energy= 0.089949
Sum of electronic and zero-point Energies= -642.535280
Sum of electronic and thermal Energies= -642.524800
Sum of electronic and thermal Enthalpies= -642.523856
Sum of electronic and thermal Free Energies= -642.572520

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.389	38.392	102.421

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.094397	-0.014485	-0.000318
2	6	0	-1.522062	-1.244433	0.000253
3	6	0	-0.151053	-1.353799	0.000480
4	6	0	0.627453	-0.192428	0.000572
5	7	0	0.020918	1.016056	0.000306
6	6	0	-1.379164	1.186417	-0.000359
7	1	0	-3.106189	0.074377	-0.000386
8	8	0	-2.416854	-2.239235	0.000367

9	1	0	0.368083	-2.306792	0.000210
10	8	0	-1.937728	2.265227	-0.000913
11	6	0	0.788806	2.284421	0.000693
12	1	0	0.519113	2.860585	-0.887318
13	1	0	0.517868	2.860680	0.888232
14	1	0	1.845445	2.025215	0.001348
15	1	0	-1.964047	-3.100249	0.000553
16	6	0	2.493052	-0.552344	-0.000223
17	8	0	2.592749	-1.764428	-0.001098
18	8	0	3.160820	0.464457	0.000263

Decarboxylation pathway for 4-protonated 1-methyl orotate r=2.0 (favored conformer, proton toward C5)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.660186849

Zero-point correction= 0.127025
(Hartree/Particle)
Thermal correction to Energy= 0.137599
Thermal correction to Enthalpy= 0.138543
Thermal correction to Gibbs Free Energy= 0.089836
Sum of electronic and zero-point Energies= -642.533162
Sum of electronic and thermal Energies= -642.522588
Sum of electronic and thermal Enthalpies= -642.521643
Sum of electronic and thermal Free Energies= -642.570351

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.345	38.624	102.513

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.112703	-0.052030	0.000151
2	6	0	1.511965	-1.269224	-0.000179
3	6	0	0.139062	-1.347755	-0.000415
4	6	0	-0.617669	-0.169679	-0.000492
5	7	0	0.022698	1.021764	-0.000286
6	6	0	1.424791	1.164496	0.000215
7	1	0	3.126133	0.013170	0.000369
8	8	0	2.386942	-2.283370	-0.000161
9	1	0	-0.392932	-2.293951	-0.000443
10	8	0	2.007217	2.231441	0.000729
11	6	0	-0.723578	2.301256	-0.000495
12	1	0	-0.448654	2.875068	0.887660
13	1	0	-0.446759	2.875815	-0.887553
14	1	0	-1.784258	2.059904	-0.001558
15	1	0	1.915365	-3.134053	-0.000300
16	6	0	-2.586303	-0.522494	0.000177
17	8	0	-2.663700	-1.728307	0.000798
18	8	0	-3.206248	0.514775	-0.000128

Decarboxylation pathway for 4-protonated 1-methyl orotate r=2.2 (favored conformer, proton toward C5)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.657366667

Zero-point correction= 0.126644
(Hartree/Particle)
Thermal correction to Energy= 0.137450
Thermal correction to Enthalpy= 0.138394
Thermal correction to Gibbs Free Energy= 0.089065
Sum of electronic and zero-point Energies= -642.530723
Sum of electronic and thermal Energies= -642.519917
Sum of electronic and thermal Enthalpies= -642.518973
Sum of electronic and thermal Free Energies= -642.568301

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.251	39.061	103.821

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.148322	-0.118849	-0.000230
2	6	0	-1.497707	-1.311252	-0.000045
3	6	0	-0.123498	-1.334790	-0.000106
4	6	0	0.600141	-0.129386	-0.000128
5	7	0	-0.104033	1.029707	-0.000201
6	6	0	-1.508195	1.122591	-0.000732
7	1	0	-3.163238	-0.094751	-0.000044
8	8	0	-2.336016	-2.359567	0.000161
9	1	0	0.429073	-2.269743	0.000033
10	8	0	-2.132730	2.167324	0.000178
11	6	0	0.595749	2.332586	0.000208
12	1	0	0.306652	2.901324	-0.887170
13	1	0	0.305826	2.901260	0.887357
14	1	0	1.663748	2.127252	0.000693
15	1	0	-1.830755	-3.190308	0.000245
16	6	0	2.773720	-0.469319	0.000098
17	8	0	2.798636	-1.663558	0.000214
18	8	0	3.296850	0.604097	0.000215

Decarboxylation pathway for 4-protonated 1-methyl orotate r=2.4 (potential energy maximum, favored conformer, proton toward C5)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.656703781

Zero-point correction= 0.126330
(Hartree/Particle)
Thermal correction to Energy= 0.137345

```
 Thermal correction to Enthalpy=                  0.138289
 Thermal correction to Gibbs Free Energy=         0.088195
 Sum of electronic and zero-point Energies=           -642.530374
 Sum of electronic and thermal Energies=              -642.519359
 Sum of electronic and thermal Enthalpies=            -642.518415
 Sum of electronic and thermal Free Energies=         -642.568509

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  86.185             39.371           105.432

                        Standard orientation:
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
    1          7             0       -2.177956   -0.173401    0.000000
    2          6             0       -1.487445   -1.343671    0.000053
    3          6             0       -0.113856   -1.321801    0.000188
    4          6             0        0.583466   -0.094941    0.000242
    5          7             0       -0.172327    1.036128    0.000126
    6          6             0       -1.576961    1.086748    0.000001
    7          1             0       -3.192878   -0.182347   -0.000078
    8          8             0       -2.293876   -2.419472   -0.000041
    9          1             0        0.457455   -2.245902    0.000192
   10          8             0       -2.236025    2.111661   -0.000090
   11          6             0        0.483279    2.360257    0.000033
   12          1             0        0.179201    2.922230    0.887090
   13          1             0        1.557042    2.187470   -0.000061
   14          1             0        0.179017    2.922211   -0.886969
   15          1             0       -1.761058   -3.232553    0.000032
   16          6             0        2.938405   -0.426512   -0.000110
   17          8             0        3.379017    0.672394   -0.000332
   18          8             0        2.909870   -1.610918    0.000022
```

5-protonated, 6-deprotonated 1-methyl uracil

B3lyp/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -454.073288246

Zero-point correction=                           0.113069
(Hartree/Particle)
 Thermal correction to Energy=                    0.121182
 Thermal correction to Enthalpy=                  0.122126
 Thermal correction to Gibbs Free Energy=         0.079661
 Sum of electronic and zero-point Energies=           -453.960219
 Sum of electronic and thermal Energies=              -453.952106
 Sum of electronic and thermal Enthalpies=            -453.951162
 Sum of electronic and thermal Free Energies=         -453.993627

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  76.043             29.384            89.375

                        Standard orientation:
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.713899	1.033691	-0.000042
2	6	0	1.699550	0.046812	-0.000272
3	6	0	1.147211	-1.363358	0.000178
4	6	0	-0.332478	-1.617800	-0.000082
5	7	0	-1.093739	-0.528270	-0.000162
6	6	0	-0.655101	0.847240	-0.000212
7	1	0	1.023588	2.002292	0.000168
8	8	0	2.878740	0.342923	-0.000082
9	1	0	1.573832	-1.900608	-0.859612
10	8	0	-1.441501	1.770709	0.000558
11	6	0	-2.568729	-0.668182	-0.000162
12	1	0	1.573182	-1.899788	0.860818
13	1	0	-2.989410	-0.190112	-0.887982
14	1	0	-2.773538	-1.736782	-0.000252
15	1	0	-2.989400	-0.190282	0.887748

5-protonated 1-methyl orotate

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.678296565

Zero-point correction= 0.127790
(Hartree/Particle)
Thermal correction to Energy= 0.138995
Thermal correction to Enthalpy= 0.139939
Thermal correction to Gibbs Free Energy= 0.089175
Sum of electronic and zero-point Energies= -642.550506
Sum of electronic and thermal Energies= -642.539301
Sum of electronic and thermal Enthalpies= -642.538357
Sum of electronic and thermal Free Energies= -642.589121

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	87.221	39.122	106.843

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.053520	0.183980	0.039179
2	6	0	-1.756689	-1.175540	-0.058451
3	6	0	-0.290039	-1.483729	-0.259101
4	6	0	0.656941	-0.336019	-0.137641
5	7	0	0.214910	0.913901	-0.109461
6	6	0	-1.177330	1.252040	0.018009
7	1	0	-3.032460	0.432839	0.158339
8	8	0	-2.626918	-2.016271	-0.002911
9	8	0	-1.536861	2.403550	0.100859
10	6	0	2.134131	-0.646298	0.052329
11	8	0	2.176501	-0.862088	1.290679

12	8	0	2.937651	-0.644217	-0.875321
13	6	0	1.154909	2.061012	-0.073561
14	1	0	0.012402	-2.272479	0.437359
15	1	0	-0.164888	-1.914359	-1.265281
16	1	0	0.711129	2.887442	-0.625801
17	1	0	1.319489	2.359232	0.964609
18	1	0	2.090079	1.745562	-0.533241

Decarboxylation pathway for 5-protonated 1-methyl orotate r=1.8

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.667631972

Zero-point correction= 0.126217
(Hartree/Particle)
Thermal correction to Energy= 0.137105
Thermal correction to Enthalpy= 0.138049
Thermal correction to Gibbs Free Energy= 0.088004
Sum of electronic and zero-point Energies= -642.541415
Sum of electronic and thermal Energies= -642.530527
Sum of electronic and thermal Enthalpies= -642.529583
Sum of electronic and thermal Free Energies= -642.579628

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.035	38.152	105.328

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.124135	0.097774	0.051071
2	6	0	-1.757792	-1.244600	-0.087698
3	6	0	-0.268164	-1.471616	-0.215212
4	6	0	0.621419	-0.281321	-0.166345
5	7	0	0.117541	0.926817	-0.068984
6	6	0	-1.302105	1.204187	0.068360
7	1	0	-3.117492	0.294495	0.148523
8	8	0	-2.593174	-2.121660	-0.102279
9	8	0	-1.705268	2.336447	0.188500
10	6	0	2.380489	-0.592537	0.054604
11	8	0	2.434207	-1.078768	1.177840
12	8	0	3.074418	-0.264969	-0.886923
13	6	0	0.983852	2.133705	-0.043353
14	1	0	0.060985	-2.166505	0.568726
15	1	0	-0.073966	-2.006621	-1.157099
16	1	0	0.555672	2.886145	-0.705143
17	1	0	1.019538	2.527840	0.974543
18	1	0	1.973765	1.837201	-0.383402

Decarboxylation pathway for 5-protonated 1-methyl orotate r=2.0

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.662399395

Zero-point correction= 0.125946
(Hartree/Particle)
Thermal correction to Energy= 0.136895
Thermal correction to Enthalpy= 0.137839
Thermal correction to Gibbs Free Energy= 0.087152
Sum of electronic and zero-point Energies= -642.536454
Sum of electronic and thermal Energies= -642.525504
Sum of electronic and thermal Enthalpies= -642.524560
Sum of electronic and thermal Free Energies= -642.575248

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.903	38.514	106.682

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.174543	-0.060731	0.008246
2	6	0	-1.663315	-1.361565	-0.059283
3	6	0	-0.155275	-1.429765	-0.087712
4	6	0	0.622139	-0.164409	-0.047653
5	7	0	-0.014579	0.979911	0.006082
6	6	0	-1.467788	1.120281	0.043247
7	1	0	-3.186988	0.035574	0.033595
8	8	0	-2.405557	-2.319301	-0.092307
9	8	0	-1.983944	2.210757	0.104633
10	6	0	2.594810	-0.488730	0.010520
11	8	0	2.672785	-1.623947	0.406855
12	8	0	3.178209	0.497696	-0.361932
13	6	0	0.708935	2.278370	0.051661
14	1	0	0.205618	-2.062876	0.735540
15	1	0	0.162081	-1.995510	-0.976304
16	1	0	0.347899	2.911396	-0.760136
17	1	0	0.497436	2.768286	1.004172
18	1	0	1.768834	2.062140	-0.059836

Decarboxylation pathway for 5-protonated 1-methyl orotate r=2.1 (potential energy maximum)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.662009438

Zero-point correction= 0.125786
(Hartree/Particle)
Thermal correction to Energy= 0.136851

```
 Thermal correction to Enthalpy=                 0.137795
 Thermal correction to Gibbs Free Energy=        0.086506
 Sum of electronic and zero-point Energies=          -642.536223
 Sum of electronic and thermal Energies=             -642.525158
 Sum of electronic and thermal Enthalpies=           -642.524214
 Sum of electronic and thermal Free Energies=        -642.575503

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  85.875             38.727           107.947

                         Standard orientation:
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
    1          7             0       -2.194810   -0.108737   -0.000110
    2          6             0       -1.645241   -1.394917   -0.000170
    3          6             0       -0.134691   -1.418159   -0.000120
    4          6             0        0.613930   -0.132900    0.000030
    5          7             0       -0.066219    0.990561    0.000080
    6          6             0       -1.520468    1.092423    0.000010
    7          1             0       -3.209750   -0.040235   -0.000150
    8          8             0       -2.359403   -2.375106   -0.000250
    9          8             0       -2.070097    2.169103    0.000050
   10          6             0        2.703190   -0.456353    0.000080
   11          8             0        2.747898   -1.652303   -0.000130
   12          8             0        3.238401    0.614247    0.000290
   13          6             0        0.619623    2.308840    0.000220
   14          1             0        0.219118   -2.012400    0.854970
   15          1             0        0.219178   -2.012220   -0.855320
   16          1             0        0.318394    2.867870   -0.887650
   17          1             0        0.318264    2.867750    0.888110
   18          1             0        1.689553    2.115339    0.000290
```

Decarboxylation pathway for 5-protonated 1-methyl orotate r=2.2

B3lyp/6-31+G*

```
SCF Done:  E(RB+HF-LYP) =  -642.662204848

Zero-point correction=                          0.125673
(Hartree/Particle)
 Thermal correction to Energy=                  0.136823
 Thermal correction to Enthalpy=                0.137768
 Thermal correction to Gibbs Free Energy=       0.086346
 Sum of electronic and zero-point Energies=          -642.536532
 Sum of electronic and thermal Energies=             -642.525381
 Sum of electronic and thermal Enthalpies=           -642.524437
 Sum of electronic and thermal Free Energies=        -642.575859

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  85.858             38.871           108.226
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.209595	-0.133297	0.000263
2	6	0	1.642629	-1.411274	-0.000109
3	6	0	0.131165	-1.412212	0.001196
4	6	0	-0.605920	-0.118032	0.000423
5	7	0	0.097354	0.993836	0.000196
6	6	0	1.550325	1.077011	0.000355
7	1	0	3.225281	-0.077913	-0.000363
8	8	0	2.343411	-2.401635	-0.001524
9	8	0	2.116725	2.145713	0.000237
10	6	0	-2.782325	-0.439370	-0.000165
11	8	0	-2.800971	-1.630536	0.000462
12	8	0	-3.275951	0.644808	-0.000952
13	6	0	-0.570895	2.320225	-0.000387
14	1	0	-0.229090	-2.003703	-0.853145
15	1	0	-0.227245	-2.001117	0.858169
16	1	0	-0.265079	2.877619	0.887129
17	1	0	-0.265065	2.876859	-0.888379
18	1	0	-1.643030	2.139593	-0.000287

Acetamide

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -209.226954130

Zero-point correction= 0.073541
(Hartree/Particle)
Thermal correction to Energy= 0.078818
Thermal correction to Enthalpy= 0.079762
Thermal correction to Gibbs Free Energy= 0.045201
Sum of electronic and zero-point Energies= -209.153413
Sum of electronic and thermal Energies= -209.148137
Sum of electronic and thermal Enthalpies= -209.147192
Sum of electronic and thermal Free Energies= -209.181753

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.365103	-0.347078	-0.000002
2	6	0	-0.074026	0.143884	-0.000028
3	8	0	-0.355569	1.336431	0.000015
4	7	0	-1.038984	-0.827036	-0.000086
5	1	0	-2.009844	-0.542770	0.000243
6	1	0	1.460448	-1.437721	-0.001103
7	1	0	1.872965	0.056118	-0.881877
8	1	0	1.872311	0.054239	0.883119
9	1	0	-0.824907	-1.812896	0.000277

1-methyl orotate acetamide complex

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -851.447424459

Zero-point correction= 0.191988
(Hartree/Particle)
Thermal correction to Energy= 0.209173
Thermal correction to Enthalpy= 0.210117
Thermal correction to Gibbs Free Energy= 0.142827
Sum of electronic and zero-point Energies= -851.255437
Sum of electronic and thermal Energies= -851.238252
Sum of electronic and thermal Enthalpies= -851.237307
Sum of electronic and thermal Free Energies= -851.304598

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.675871	-0.041277	0.063035
2	6	0	4.156486	-0.139702	0.008643
3	8	0	3.462380	0.881724	0.009291
4	7	0	3.624429	-1.382637	-0.039750
5	7	0	-1.379838	-0.802044	-0.068332
6	6	0	-0.013114	-0.591593	-0.062633
7	7	0	0.394184	0.716250	-0.012744
8	6	0	-0.440486	1.859866	0.028099
9	6	0	-1.843808	1.544335	0.020936
10	6	0	-2.284987	0.254226	-0.010778
11	8	0	0.800759	-1.536162	-0.103922
12	8	0	0.071483	2.981404	0.064175
13	6	0	-1.870854	-2.187000	-0.112084
14	1	0	2.598210	-1.488750	-0.067130
15	1	0	6.180155	-1.013844	0.043496
16	1	0	6.020593	0.557274	-0.786480
17	1	0	5.961611	0.490575	0.976595
18	1	0	-2.648100	-2.265375	-0.875908
19	1	0	-1.030241	-2.833578	-0.356817
20	1	0	-2.302483	-2.457887	0.854234
21	6	0	-3.786079	-0.112900	0.055015
22	8	0	-4.442167	0.140679	-0.978773
23	8	0	-4.126407	-0.625055	1.148467
24	1	0	-2.554257	2.361030	0.039580
25	1	0	1.407540	0.877767	-0.008124
26	1	0	4.208989	-2.204651	-0.028955

ONSAGER

6-deprotonated 1-methyl uracil

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -453.558923424

Zero-point correction= (Hartree/Particle)	0.100846
Thermal correction to Energy=	0.108480
Thermal correction to Enthalpy=	0.109424
Thermal correction to Gibbs Free Energy=	0.068517
Sum of electronic and zero-point Energies=	-453.458078
Sum of electronic and thermal Energies=	-453.450443
Sum of electronic and thermal Enthalpies=	-453.449499
Sum of electronic and thermal Free Energies=	-453.490406

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.068698	-0.514797	-0.000020
2	6	0	-0.658889	0.810380	-0.000005
3	7	0	0.714308	0.980623	-0.000012
4	6	0	1.693769	-0.031080	0.000003
5	6	0	1.131358	-1.348690	0.000003
6	6	0	-0.228857	-1.639135	-0.000006
7	6	0	-2.521696	-0.702404	-0.000007
8	8	0	-1.430583	1.777616	0.000024
9	1	0	1.036589	1.941216	0.000008
10	8	0	2.898699	0.308662	0.000011
11	1	0	1.851561	-2.165988	0.000012
12	1	0	-2.694207	-1.778375	-0.000147
13	1	0	-2.976109	-0.241270	0.884710
14	1	0	-2.976149	-0.241017	-0.884568

1-methyl orotate

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.212109454

Zero-point correction= (Hartree/Particle)	0.116156
Thermal correction to Energy=	0.126794
Thermal correction to Enthalpy=	0.127738
Thermal correction to Gibbs Free Energy=	0.078434
Sum of electronic and zero-point Energies=	-642.095954
Sum of electronic and thermal Energies=	-642.085316
Sum of electronic and thermal Enthalpies=	-642.084372
Sum of electronic and thermal Free Energies=	-642.133676

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.564	37.632	103.769

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.117932	0.923821	-0.073458
2	6	0	-1.255512	1.188861	-0.045290
3	7	0	-2.058773	0.063945	0.029352
4	6	0	-1.655652	-1.282080	0.063281
5	6	0	-0.226186	-1.444014	0.021337
6	6	0	0.615522	-0.368902	-0.026762
7	6	0	1.019860	2.081114	-0.156185
8	8	0	-1.729243	2.319726	-0.084529
9	1	0	-3.056482	0.247540	0.049888
10	8	0	-2.506647	-2.176489	0.122832
11	1	0	0.179153	-2.447373	0.021797
12	6	0	2.150775	-0.576051	0.034926
13	8	0	2.643267	-1.245711	-0.904687
14	8	0	2.699619	-0.071089	1.045388
15	1	0	1.739789	1.923553	-0.963726
16	1	0	0.410004	2.959359	-0.361889
17	1	0	1.564617	2.197493	0.782791

2-protonated, 6-deprotonated 1-methyl uracil (favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -454.047688581

Zero-point correction= 0.112999
(Hartree/Particle)
Thermal correction to Energy= 0.120994
Thermal correction to Enthalpy= 0.121938
Thermal correction to Gibbs Free Energy= 0.080532
Sum of electronic and zero-point Energies= -453.934690
Sum of electronic and thermal Energies= -453.926694
Sum of electronic and thermal Enthalpies= -453.925750
Sum of electronic and thermal Free Energies= -453.967157

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.925	30.079	87.147

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.704103	0.981459	-0.000100
2	6	0	-1.733650	-0.017515	-0.000100
3	6	0	-1.189790	-1.345139	-0.000100
4	6	0	0.148625	-1.685151	0.000115
5	7	0	1.032065	-0.550182	0.000169
6	6	0	0.606277	0.710909	0.000027
7	1	0	-0.991728	1.956021	-0.000206
8	8	0	-2.906757	0.361483	-0.000527
9	1	0	-1.927664	-2.144026	-0.000298

10	8	0	1.389991	1.786109	0.000070
11	6	0	2.485537	-0.810325	0.000395
12	1	0	2.592196	-1.893432	0.000274
13	1	0	2.961557	-0.404977	-0.900292
14	1	0	2.961227	-0.405216	0.901364
15	1	0	2.340811	1.575277	0.000308

2-protonated 1-methyl orotate (favored conformer, proton toward N1-methyl)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.675650378

Zero-point correction= 0.128279
(Hartree/Particle)
Thermal correction to Energy= 0.138912
Thermal correction to Enthalpy= 0.139857
Thermal correction to Gibbs Free Energy= 0.091357
Sum of electronic and zero-point Energies= -642.547371
Sum of electronic and thermal Energies= -642.536738
Sum of electronic and thermal Enthalpies= -642.535794
Sum of electronic and thermal Free Energies= -642.584293

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.169	39.290	102.075

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.040935	-0.160342	-0.050409
2	6	0	1.476285	-1.472846	-0.061282
3	6	0	0.034762	-1.444124	0.011286
4	6	0	-0.693360	-0.299786	0.046293
5	7	0	-0.016684	0.950448	0.043009
6	6	0	1.327713	0.969261	0.018396
7	1	0	3.058306	-0.077867	-0.071513
8	8	0	2.202978	-2.447706	-0.124912
9	1	0	-0.495959	-2.385585	0.041605
10	8	0	2.051486	2.062568	0.062756
11	6	0	-2.268332	-0.431454	-0.014106
12	8	0	-2.875378	0.509494	-0.569638
13	8	0	-2.689901	-1.511288	0.452308
14	6	0	-0.724468	2.254757	0.151260
15	1	0	-1.787755	2.047788	0.041675
16	1	0	-0.509832	2.714528	1.121215
17	1	0	-0.421813	2.909112	-0.672237
18	1	0	1.558227	2.901881	0.115859

4-protonated, 6-deprotonated 1-methyl uracil (favored conformer, proton toward C5)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -454.064847101

Zero-point correction= (Hartree/Particle)	0.113757
Thermal correction to Energy=	0.121598
Thermal correction to Enthalpy=	0.122542
Thermal correction to Gibbs Free Energy=	0.081457
Sum of electronic and zero-point Energies=	-453.951090
Sum of electronic and thermal Energies=	-453.943249
Sum of electronic and thermal Enthalpies=	-453.942305
Sum of electronic and thermal Free Energies=	-453.983390

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.304	29.639	86.470

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.679978	0.980696	-0.000004
2	6	0	1.562308	-0.057292	-0.000040
3	6	0	1.088630	-1.348974	-0.000045
4	6	0	-0.301519	-1.633263	-0.000014
5	7	0	-1.106229	-0.520091	0.000021
6	6	0	-0.700730	0.820962	0.000029
7	1	0	1.025996	1.935087	0.000000
8	8	0	2.835404	0.363437	-0.000067
9	1	0	1.797343	-2.172986	-0.000074
10	8	0	-1.463535	1.778856	0.000061
11	6	0	-2.566747	-0.698146	0.000055
12	1	0	-2.744075	-1.772234	0.000046
13	1	0	-3.005666	-0.230676	0.887316
14	1	0	-3.005710	-0.230653	-0.887171
15	1	0	3.449263	-0.390843	-0.000092

4-protonated 1-methyl orotate (favored conformer, proton toward C5)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.686025156

Zero-point correction= (Hartree/Particle)	0.128437
Thermal correction to Energy=	0.139450
Thermal correction to Enthalpy=	0.140394
Thermal correction to Gibbs Free Energy=	0.090112
Sum of electronic and zero-point Energies=	-642.557589
Sum of electronic and thermal Energies=	-642.546575
Sum of electronic and thermal Enthalpies=	-642.545631
Sum of electronic and thermal Free Energies=	-642.595914

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.506	39.329	105.829

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.020369	0.252843	-0.002614
2	6	0	1.682438	-1.060806	0.013964
3	6	0	0.344978	-1.421896	0.012673
4	6	0	-0.616644	-0.410054	-0.005790
5	7	0	-0.238754	0.895918	-0.034330
6	6	0	1.108493	1.309271	-0.016252
7	1	0	3.004758	0.515389	0.005668
8	8	0	2.737035	-1.861186	0.030230
9	1	0	0.040297	-2.461003	0.022093
10	8	0	1.462412	2.468634	-0.015329
11	6	0	-1.254289	1.966765	-0.040877
12	1	0	-0.756285	2.897080	-0.306408
13	1	0	-2.020535	1.712183	-0.774347
14	1	0	-1.703405	2.044280	0.952147
15	1	0	2.497468	-2.804396	0.041763
16	6	0	-2.130982	-0.715122	0.013307
17	8	0	-2.613320	-0.940038	-1.113858
18	8	0	-2.628322	-0.661635	1.155899

5-protonated, 6-deprotonated 1-methyl uracil

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -454.073693767

Zero-point correction= 0.112936
(Hartree/Particle)
Thermal correction to Energy= 0.121080
Thermal correction to Enthalpy= 0.122025
Thermal correction to Gibbs Free Energy= 0.079423
Sum of electronic and zero-point Energies= -453.960758
Sum of electronic and thermal Energies= -453.952613
Sum of electronic and thermal Enthalpies= -453.951669
Sum of electronic and thermal Free Energies= -453.994271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.979	29.439	89.662

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.716938	1.030702	0.000089
2	6	0	1.699855	0.045329	-0.000093
3	6	0	1.144544	-1.363888	0.000197
4	6	0	-0.335657	-1.616510	-0.000026

5	7	0	-1.096566	-0.527194	-0.000022
6	6	0	-0.655275	0.846145	0.000163
7	1	0	1.024414	1.999840	0.000021
8	8	0	2.881378	0.339573	-0.000311
9	1	0	1.569314	-1.901570	-0.860159
10	8	0	-1.434578	1.774511	0.000161
11	6	0	-2.572774	-0.665511	-0.000184
12	1	0	1.568807	-1.900986	0.861186
13	1	0	-2.992133	-0.186961	-0.888142
14	1	0	-2.779260	-1.733699	-0.000370
15	1	0	-2.992296	-0.187245	0.887850

5-protonated 1-methyl orotate

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.684867538

Zero-point correction= 0.127564
(Hartree/Particle)
Thermal correction to Energy= 0.138881
Thermal correction to Enthalpy= 0.139825
Thermal correction to Gibbs Free Energy= 0.088358
Sum of electronic and zero-point Energies= -642.557304
Sum of electronic and thermal Energies= -642.545987
Sum of electronic and thermal Enthalpies= -642.545042
Sum of electronic and thermal Free Energies= -642.596510

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.149	39.140	108.322

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.087290	0.128352	0.002737
2	6	0	-1.733236	-1.219285	-0.035011
3	6	0	-0.246209	-1.479584	-0.160409
4	6	0	0.663409	-0.301639	-0.072077
5	7	0	0.182090	0.920069	-0.047580
6	6	0	-1.247437	1.221508	0.009105
7	1	0	-3.081514	0.346221	0.065078
8	8	0	-2.557668	-2.102591	0.016529
9	8	0	-1.617500	2.364361	0.067243
10	6	0	2.165139	-0.591050	0.030164
11	8	0	2.457565	-0.831762	1.219897
12	8	0	2.802104	-0.575245	-1.034036
13	6	0	1.060064	2.114061	-0.003914
14	1	0	0.053742	-2.211623	0.597833
15	1	0	-0.063778	-1.966997	-1.130050
16	1	0	0.638568	2.875500	-0.658744
17	1	0	1.092117	2.496783	1.018515
18	1	0	2.050875	1.819007	-0.342949

Decarboxylation pathway for 5-protonated 1-methyl orotate r=2.3 (potential energy maximum)

B3lyp/6-31+G*

SCF Done: E(RB+HF-LYP) = -642.664021354

Zero-point correction= (Hartree/Particle)	0.125453
Thermal correction to Energy=	0.136689
Thermal correction to Enthalpy=	0.137633
Thermal correction to Gibbs Free Energy=	0.085926
Sum of electronic and zero-point Energies=	-642.538569
Sum of electronic and thermal Energies=	-642.527332
Sum of electronic and thermal Enthalpies=	-642.526388
Sum of electronic and thermal Free Energies=	-642.578096

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.774	39.038	108.827

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.223159	-0.155742	-0.000006
2	6	0	-1.639842	-1.423063	0.000019
3	6	0	-0.127061	-1.405410	0.000056
4	6	0	0.598100	-0.103317	0.000030
5	7	0	-0.119495	0.997498	0.000002
6	6	0	-1.577214	1.063639	-0.000015
7	1	0	-3.240053	-0.110365	-0.000025
8	8	0	-2.320044	-2.428364	0.000014
9	8	0	-2.151476	2.125376	-0.000039
10	6	0	2.828914	-0.421967	-0.000006
11	8	0	2.844507	-1.612910	-0.000138
12	8	0	3.310882	0.665169	0.000102
13	6	0	0.528266	2.333720	-0.000016
14	1	0	0.234989	-1.990746	0.857483
15	1	0	0.235041	-1.990817	-0.857299
16	1	0	0.213844	2.887056	-0.887005
17	1	0	0.213821	2.887091	0.886943
18	1	0	1.603005	2.169716	0.000005