Supporting Information **INFORMATION**

^{13}C Kinetic Isotope Effects and the Mechanism of the Uncatalyzed Decarboxylation of Orotic Acid

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The structures reported here were obtained with Gaussian 94[1] or Gaussian 98.[2]

Contents

1-Methylorotic acid

SCF Done: E(RB+HF-LYP) = -642.716482983

Zero-point correction=	0.129751 (Hartree/Particle)
Thermal correction to Energy=	0.140324
Thermal correction to Enthalpy=	0.141268
Thermal correction to Gibbs Free Energy=	0.092813
Sum of electronic and zero-point Energies=	-642.586732
Sum of electronic and thermal Energies=	-642.576159
Sum of electronic and thermal Enthalpies=	-642.575215
Sum of electronic and thermal Free Energies=	-642.623670

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	88.055	38.769	101.982

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.012235	0.983006	-0.064625
2	6	0	1.384620	1.119857	-0.008971
3	7	0	2.090308	-0.071449	0.056114
4	6	0	1.587152	-1.377572	0.049380
5	6	0	0.132676	-1.422632	0.002335
6	6	0	-0.595729	-0.275480	-0.034440
7	6	0	-0.783431	2.230796	-0.230256
8	8	0	1.949092	2.202455	-0.023078
9	1	0	3.099915	0.031073	0.095555
10	8	0	2.333478	-2.346117	0.088648
11	1	0	-0.347267	-2.390642	0.022534
12	6	0	-2.092594	-0.364919	0.082149
13	8	0	-2.568493	-1.507985	-0.456120
14	8	0	-2.799197	0.455972	0.626447
15	1	0	-1.273759	2.511006	0.703103
16	1	0	-0.075338	3.003302	-0.523615
17	1	0	-1.537136	2.101239	-1.008457
18	1	0	-3.528132	-1.531769	-0.277902

1-methylorotate

SCF Done: E(RB+HF-LYP) = -642.206011223

Zero-point correction=	0.116180 (Hartree/Particle)
Thermal correction to Energy=	0.126891
Thermal correction to Enthalpy=	0.127835
Thermal correction to Gibbs Free Energy=	0.078093
Sum of electronic and zero-point Energies=	-642.089831
Sum of electronic and thermal Energies=	-642.079120
Sum of electronic and thermal Enthalpies=	-642.078176
Sum of electronic and thermal Free Energies=	-642.127918

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	79.625	37.676	104.691

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.146491	0.900960	-0.050300
2	6	0	-1.207227	1.215519	-0.037387
3	7	0	-2.048230	0.121646	0.012960

4	6	0	-1.697094	-1.245951	0.043602
5	6	0	-0.278746	-1.460627	0.023324
6	6	0	0.598783	-0.412135	-0.010302
7	6	0	1.109360	2.010692	-0.088365
8	8	0	-1.647654	2.367680	-0.069601
9	1	0	-3.038699	0.335616	0.022376
10	8	0	-2.597247	-2.093209	0.081574
11	1	0	0.091030	-2.478001	0.030465
12	6	0	2.130633	-0.621541	0.024673
13	8	0	2.631424	-1.036767	-1.043220
14	8	0	2.650461	-0.332468	1.128510
15	1	0	1.811829	1.850556	-0.910572
16	1	0	0.549152	2.931584	-0.241511
17	1	0	1.668743	2.044376	0.849242

decarboxylation pathway for 1-methylorotate with r = 3.55Å (approximate free energy maximum)

SCF Done: E(RB+HF-LYP) = -642.153906885

Zero-point correction=	0.112852 (Hartree/Particle)
Thermal correction to Energy=	0.124184
Thermal correction to Enthalpy=	0.125128
Thermal correction to Gibbs Free Energy=	0.071699
Sum of electronic and zero-point Energies=	-642.041055
Sum of electronic and thermal Energies=	-642.029723
Sum of electronic and thermal Enthalpies=	-642.028779
Sum of electronic and thermal Free Energies=	-642.082208

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	77.926	38.095	112.450

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.503048	-0.955738	-0.000003
2	6	0	-1.887138	-0.974585	0.000002
3	7	0	-2.470240	0.275170	0.000003
4	6	0	-1.809577	1.525191	-0.000001
5	6	0	-0.379498	1.398299	-0.000007
6	6	0	0.306680	0.194652	-0.000008
7	6	0	0.131950	-2.273127	-0.000003
8	8	0	-2.568439	-2.013464	0.000007
9	1	0	-3.483246	0.292140	0.000007
10	8	0	-2.506848	2.556978	0.000000
11	1	0	0.177335	2.332373	-0.000011
12	6	0	3.855448	0.288199	0.000002
13	8	0	3.847238	1.457952	0.000009
14	8	0	3.968969	-0.877754	-0.000004
15	1	0	-0.161725	-2.850851	0.885527
16	1	0	-0.161735	-2.850856	-0.885525
17	1	0	1.207835	-2.100290	-0.000010

1-methyluracil anion

SCF Done: E(RB+HF-LYP) = -453.556115604

Zero-point correction=	0.100927 (Hartree/Particle)
Thermal correction to Energy=	0.108560
Thermal correction to Enthalpy=	0.109504
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	86.094

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.065170	-0.511429	-0.000058
2	6	0	-0.659113	0.811319	0.000008
3	7	0	0.709021	0.982496	-0.000087
4	6	0	1.694949	-0.031382	-0.000018
5	6	0	1.133990	-1.351894	0.000088
6	6	0	-0.223132	-1.641334	0.000076
7	6	0	-2.513480	-0.710467	-0.000086
8	8	0	-1.438676	1.779893	0.000136
9	1	0	1.036742	1.941110	-0.000053
10	8	0	2.891892	0.316300	-0.000042
11	1	0	1.854119	-2.167348	0.000179
12	1	0	-2.974495	-0.255029	0.885833
13	1	0	-2.974452	-0.254468	-0.885763
14	1	0	-2.673889	-1.788728	-0.000348

1-methylorotate 2-protonated, isomer 1 (disfavored isomer)

SCF Done: E(RB+HF-LYP) = -642.644861284

Zero-point correction=	0.127583 (Hartree/Particle)
Thermal correction to Energy=	0.138849
Thermal correction to Enthalpy=	0.139794
Thermal correction to Gibbs Free Energy=	0.089394
Sum of electronic and zero-point Energies=	-642.517279
Sum of electronic and thermal Energies=	-642.506012
Sum of electronic and thermal Enthalpies=	-642.505068
Sum of electronic and thermal Free Energies=	-642.555467

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	87.129	40.201	106.074

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.136750	0.871172	-0.073410
2	6	0	-1.172107	1.082429	-0.033155
3	7	0	-2.025616	0.057478	0.033310
4	6	0	-1.642254	-1.352796	0.041867
5	6	0	-0.220590	-1.514039	-0.003067
6	6	0	0.635779	-0.452982	-0.032609

7	6	0	1.096884	2.005409	-0.146055
8	8	0	-1.601155	2.344875	-0.063219
9	1	0	-3.029096	0.212134	0.071806
10	8	0	-2.541054	-2.171469	0.084134
11	1	0	0.178693	-2.520973	-0.008419
12	6	0	2.176744	-0.588450	0.044607
13	8	0	2.713993	-1.059405	-0.968480
14	8	0	2.603762	-0.170688	1.142326
15	1	0	1.815174	1.781240	-0.935636
16	1	0	0.555484	2.919684	-0.374956
17	1	0	1.621898	2.072772	0.806879
18	1	0	-2.571182	2.410664	-0.066592

1-methylorotate 2-protonated, isomer 2 (favored isomer)

E(RB+HF-LYP) = -642.647672202

Zero-point correction=	0.127864 (Hartree/Particle)
Thermal correction to Energy=	0.138627
Thermal correction to Enthalpy=	0.139571
Thermal correction to Gibbs Free Energy=	0.090609
Sum of electronic and zero-point Energies=	-642.519808
Sum of electronic and thermal Energies=	-642.509045
Sum of electronic and thermal Enthalpies=	-642.508101
Sum of electronic and thermal Free Energies=	-642.557064

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.990	39.562	103.050

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.072320	0.915651	-0.042865
2	6	0	-1.256263	1.021592	-0.038425
3	7	0	-2.039035	-0.050629	0.046158
4	6	0	-1.560383	-1.417043	0.083377
5	6	0	-0.123848	-1.480824	0.014230
6	6	0	0.669367	-0.376928	-0.028718
7	6	0	0.887575	2.152183	-0.144983
8	8	0	-1.892399	2.185540	-0.123785
9	1	0	-3.047323	0.081537	0.051412
10	8	0	-2.382576	-2.309398	0.153452
11	1	0	0.348592	-2.454984	-0.016368
12	6	0	2.233571	-0.522221	0.019607
13	8	0	2.661201	-1.444853	-0.682100
14	8	0	2.781762	0.295966	0.795965
15	1	0	1.918490	1.859601	0.073080
16	1	0	0.798103	2.579380	-1.149388
17	1	0	0.580521	2.864834	0.628124
18	1	0	-1.275396	2.935891	-0.188685

decarboxylation pathway for 1-methylorotate 2-protonated, isomer 1 (disfavored isomer) r = 2.2Å (approximate free energy maximum)

SCF Done: E(RB+HF-LYP) = -642.629071393

Zero-point correction=	0.125486 (Hartree/Particle)

Thermal correction to Energy= 0.136633
Thermal correction to Enthalpy= 0.137577
Thermal correction to Gibbs Free Energy= 0.087428
Sum of electronic and zero-point Energies= -642.503585
Sum of electronic and thermal Energies= -642.492438
Sum of electronic and thermal Enthalpies= -642.491494
Sum of electronic and thermal Free Energies= -642.541644

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	85.738	39.859	105.548

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.184125	0.958857	0.000021
2	6	0	1.509366	0.902413	-0.000003
3	7	0	2.138682	-0.276031	-0.000041
4	6	0	1.464445	-1.570015	-0.000026
5	6	0	0.034785	-1.416978	0.000059
6	6	0	-0.615792	-0.215658	0.000082
7	6	0	-0.475023	2.286550	0.000068
8	8	0	2.180966	2.060316	0.000026
9	1	0	3.153058	-0.332434	-0.000070
10	8	0	2.172656	-2.561974	-0.000081
11	1	0	-0.557256	-2.326681	0.000101
12	6	0	-2.812717	-0.331944	-0.000025
13	8	0	-2.968905	-1.513063	0.000154
14	8	0	-3.224332	0.793110	-0.000233
15	1	0	-0.184148	2.846656	0.892586
16	1	0	-0.183372	2.847118	-0.891900
17	1	0	-1.546728	2.098912	-0.000420
18	1	0	3.145327	1.933326	-0.000014

decarboxylation pathway for 1-methylorotate 2-protonated, isomer 2 (favored isomer) r = 2.2Å (approximate free energy maximum)

SCF Done: E(RB+HF-LYP) = -642.629071384
Zero-point correction= 0.125485 (Hartree/Particle)
Thermal correction to Energy= 0.136632
Thermal correction to Enthalpy= 0.137576
Thermal correction to Gibbs Free Energy= 0.087424
Sum of electronic and zero-point Energies= -642.503586
Sum of electronic and thermal Energies= -642.492439
Sum of electronic and thermal Enthalpies= -642.491495
Sum of electronic and thermal Free Energies= -642.541647

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	85.738	39.859	105.554

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.184216	0.958896	0.000014
2	6	0	1.509449	0.902343	-0.000006
3	7	0	2.138667	-0.276154	-0.000041
4	6	0	1.464315	-1.570081	-0.000020
5	6	0	0.034671	-1.416921	0.000043

6	6	0	-0.615821	-0.215551	0.000060
7	6	0	-0.474836	2.286634	0.000070
8	8	0	2.181144	2.060193	0.000018
9	1	0	3.153038	-0.332644	-0.000062
10	8	0	2.172443	-2.562100	-0.000056
11	1	0	-0.557454	-2.326572	0.000077
12	6	0	-2.812745	-0.331850	-0.000020
13	8	0	-2.968921	-1.512964	0.000130
14	8	0	-3.224392	0.793183	-0.000197
15	1	0	-0.183869	2.846752	0.892551
16	1	0	-0.183219	2.847160	-0.891937
17	1	0	-1.546555	2.099054	-0.000339
18	1	0	3.145493	1.933117	-0.000015

decarboxylation pathway for 1-methylorotate 2-protonated, isomer 2 (favored isomer) r = 2.411Å (potential energy maximum)

SCF Done: E(RB+HF-LYP) = -642.628093044

Zero-point correction=	0.125071 (Hartree/Particle)
Thermal correction to Energy=	0.136486
Thermal correction to Enthalpy=	0.137430
Thermal correction to Gibbs Free Energy=	0.086306
Sum of electronic and zero-point Energies=	-642.503022
Sum of electronic and thermal Energies=	-642.491607
Sum of electronic and thermal Enthalpies=	-642.490663
Sum of electronic and thermal Free Energies=	-642.541787

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	85.646	40.243	107.600

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.246476	-0.959725	0.000000
2	6	0	-1.569205	-0.880053	0.000000
3	7	0	-2.175919	0.310252	-0.000001
4	6	0	-1.473979	1.588897	-0.000001
5	6	0	-0.048493	1.405638	0.000000
6	6	0	0.594689	0.194585	0.000000
7	6	0	0.386414	-2.297071	0.000000
8	8	0	-2.266931	-2.025028	0.000002
9	1	0	-3.188737	0.387392	0.000001
10	8	0	-2.163570	2.595893	-0.000001
11	1	0	0.549664	2.311835	0.000001
12	6	0	3.003517	0.301422	0.000000
13	8	0	3.085681	1.479140	0.000003
14	8	0	3.323241	-0.840163	-0.000003
15	1	0	0.089295	-2.855672	0.891907
16	1	0	0.089294	-2.855673	-0.891906
17	1	0	1.460360	-2.125766	0.000000
18	1	0	-3.228129	-1.875044	0.000001

decarboxylation pathway for 1-methylorotate 2-protonated, isomer 2 (favored isomer) pi complex with r = 2.907

SCF Done: E(RB+HF-LYP) = -642.628998294

Zero-point correction=	0.124766 (Hartree/Particle)
Thermal correction to Energy=	0.137369
Thermal correction to Enthalpy=	0.138313
Thermal correction to Gibbs Free Energy=	0.083041
Sum of electronic and zero-point Energies=	-642.504233
Sum of electronic and thermal Energies=	-642.491630
Sum of electronic and thermal Enthalpies=	-642.490685
Sum of electronic and thermal Free Energies=	-642.545957

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.200	42.476	116.329

1	7	0	0.365811	-0.952446	0.000055
2	6	0	1.686055	-0.856579	0.000061
3	7	0	2.277379	0.341626	0.000008
4	6	0	1.556024	1.608495	-0.000055
5	6	0	0.134432	1.403702	-0.000052
6	6	0	-0.510390	0.186835	-0.000001
7	6	0	-0.245910	-2.296644	0.000116
8	8	0	2.404252	-1.991818	0.000123
9	1	0	3.288784	0.433204	0.000011
10	8	0	2.232849	2.626404	-0.000098
11	1	0	-0.465030	2.309589	-0.000095
12	6	0	-3.416854	0.263085	-0.000066
13	8	0	-3.399305	1.432808	-0.000087
14	8	0	-3.574900	-0.899315	-0.000049
15	1	0	0.054758	-2.854452	-0.891641
16	1	0	0.054672	-2.854329	0.891980
17	1	0	-1.321419	-2.133092	0.000056
18	1	0	3.362590	-1.823176	0.000120

1-methyluracil 2-protonated zwitterion isomer 1 (disfavored isomer)

SCF Done: E(RB+HF-LYP) = -454.031896644

Zero-point correction=	0.112277 (Hartree/Particle)
Thermal correction to Energy=	0.119901
Thermal correction to Enthalpy=	0.120845
Thermal correction to Gibbs Free Energy=	0.080105
Sum of electronic and zero-point Energies=	-453.919619
Sum of electronic and thermal Energies=	-453.911996
Sum of electronic and thermal Enthalpies=	-453.911052
Sum of electronic and thermal Free Energies=	-453.951792

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	75.239	28.745	85.745

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.039327	-0.533092	-0.000282
2	6	0	-0.613422	0.718949	-0.000081
3	7	0	0.699335	0.977993	-0.000083
4	6	0	1.736388	-0.043592	0.000096
5	6	0	1.174769	-1.365068	0.000304
6	6	0	-0.166455	-1.680610	0.000189
7	6	0	-2.482226	-0.838226	-0.000206
8	8	0	-1.509237	1.723909	0.000303

9	1	0	1.049912	1.930856	-0.000013
10	8	0	2.895198	0.348984	-0.000258
11	1	0	1.901607	-2.172528	0.000521
12	1	0	-2.699320	-1.433303	0.888766
13	1	0	-3.078808	0.074042	-0.005106
14	1	0	-2.697027	-1.441572	-0.884068
15	1	0	-1.078426	2.596344	0.000284

1-methyluracil 2-protonated zwitterion isomer 2 (favored isomer)

E(RB+HF-LYP) = -454.034797909

Zero-point correction=	0.112665 (Hartree/Particle)
Thermal correction to Energy=	0.120825
Thermal correction to Enthalpy=	0.121769
Thermal correction to Gibbs Free Energy=	0.079945
Sum of electronic and zero-point Energies=	-453.922133
Sum of electronic and thermal Energies=	-453.913973
Sum of electronic and thermal Enthalpies=	-453.913029
Sum of electronic and thermal Free Energies=	-453.954853

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	75.819	30.399	88.025

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.026457	-0.545484	0.000012
2	6	0	0.604612	0.713757	-0.000085
3	7	0	-0.696660	0.988798	-0.000113
4	6	0	-1.740816	-0.018149	0.000002
5	6	0	-1.194939	-1.349939	-0.000123
6	6	0	0.140025	-1.689486	-0.000023
7	6	0	2.469909	-0.821122	0.000101
8	8	0	1.414545	1.786245	-0.000022
9	1	0	-0.995632	1.959470	0.000012
10	8	0	-2.898146	0.377009	0.000171
11	1	0	-1.932409	-2.147502	-0.000191
12	1	0	2.556182	-1.907258	-0.000099
13	1	0	2.954451	-0.424459	-0.901850
14	1	0	2.954266	-0.424819	0.902311
15	1	0	2.350626	1.524975	0.000106

1-methylorotate 4-protonated, isomer 1 (disfavored isomer)

SCF Done: E(RB+HF-LYP) = -642.664946981

Zero-point correction=	0.127504 (Hartree/Particle)
Thermal correction to Energy=	0.138989
Thermal correction to Enthalpy=	0.139933
Thermal correction to Gibbs Free Energy=	0.088544
Sum of electronic and zero-point Energies=	-642.537443
Sum of electronic and thermal Energies=	-642.525958
Sum of electronic and thermal Enthalpies=	-642.525014
Sum of electronic and thermal Free Energies=	-642.576403

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN

TOTAL	87.217	40.234	108.157

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.047504	0.967515	0.061120
2	6	0	1.342629	1.100317	0.077938
3	7	0	2.031949	-0.121091	-0.006470
4	6	0	1.434122	-1.345732	-0.100728
5	6	0	0.065153	-1.424922	-0.115175
6	6	0	-0.675479	-0.238021	-0.032685
7	6	0	-0.853397	2.208192	0.142914
8	8	0	1.949949	2.150231	0.157036
9	1	0	3.040790	-0.010632	0.006179
10	8	0	2.193004	-2.444071	-0.177346
11	1	0	-0.434278	-2.381698	-0.188889
12	6	0	-2.211171	-0.260853	-0.047382
13	8	0	-2.701518	-0.357634	1.091071
14	8	0	-2.679421	-0.173473	-1.195992
15	1	0	-1.515536	2.135107	1.007593
16	1	0	-0.170913	3.048635	0.244792
17	1	0	-1.449150	2.297888	-0.767591
18	1	0	3.147034	-2.260015	-0.156384

1-methylorotate 4-protonated, isomer 2 (favored isomer)

SCF Done: E(RB+HF-LYP) = -642.672851753

Zero-point correction=	0.128086 (Hartree/Particle)
Thermal correction to Energy=	0.138446
Thermal correction to Enthalpy=	0.139391
Thermal correction to Gibbs Free Energy=	0.090813
Sum of electronic and zero-point Energies=	-642.544766
Sum of electronic and thermal Energies=	-642.534405
Sum of electronic and thermal Enthalpies=	-642.533461
Sum of electronic and thermal Free Energies=	-642.582039

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.876	37.677	102.240

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.233039	0.919117	-0.004750
2	6	0	-1.115386	1.309782	-0.001831
3	7	0	-2.013199	0.237236	-0.000357
4	6	0	-1.653531	-1.073298	0.001355
5	6	0	-0.324041	-1.413908	0.000823
6	6	0	0.626431	-0.381174	-0.001436
7	6	0	1.254110	1.992360	-0.004724
8	8	0	-1.505823	2.459832	-0.001074
9	1	0	-2.996636	0.489875	0.001240
10	8	0	-2.703492	-1.901764	0.003363
11	1	0	0.006477	-2.445639	0.001774
12	6	0	2.129253	-0.702343	0.001494
13	8	0	2.597406	-0.820303	-1.144256
14	8	0	2.596496	-0.789708	1.150500
15	1	0	1.897081	1.860475	-0.876925
16	1	0	0.737944	2.948693	-0.043563
17	1	0	1.850195	1.908488	0.906164

18	1	0	-2.411645	-2.829334	0.004709

decarboxylation pathway for 1-methylorotate 4-protonated, isomer 2 (favored isomer) r = 2.2Å (approximate free energy maximum)

SCF Done: E(RB+HF-LYP) = -642.657366865

Zero-point correction=	0.126644 (Hartree/Particle)
Thermal correction to Energy=	0.137451
Thermal correction to Enthalpy=	0.138395
Thermal correction to Gibbs Free Energy=	0.089060
Sum of electronic and zero-point Energies=	-642.530723
Sum of electronic and thermal Energies=	-642.519916
Sum of electronic and thermal Enthalpies=	-642.518972
Sum of electronic and thermal Free Energies=	-642.568307

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.252	39.061	103.834

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.104141	1.029835	0.000008
2	6	0	1.508247	1.122550	0.000022
3	7	0	2.148200	-0.119031	0.000018
4	6	0	1.497518	-1.311376	0.000000
5	6	0	0.123244	-1.334756	-0.000012
6	6	0	-0.600009	-0.129212	-0.000008
7	6	0	-0.595587	2.332754	0.000011
8	8	0	2.133028	2.167140	0.000037
9	1	0	3.163121	-0.095038	0.000024
10	8	0	2.335769	-2.359718	-0.000003
11	1	0	-0.429540	-2.269560	-0.000024
12	6	0	-2.773581	-0.469194	-0.000024
13	8	0	-2.798507	-1.663431	-0.000023
14	8	0	-3.297017	0.604071	-0.000027
15	1	0	-0.306046	2.901423	0.887288
16	1	0	-0.306023	2.901439	-0.887249
17	1	0	-1.663591	2.127485	-0.000004
18	1	0	1.830502	-3.190455	-0.000020

decarboxylation pathway for 1-methylorotate 4-protonated, isomer 2 (favored isomer) r = 2.378Å (potential energy maximum)

SCF Done: E(RB+HF-LYP) = -642.656703805

Zero-point correction=	0.126329 (Hartree/Particle)
Thermal correction to Energy=	0.137345
Thermal correction to Enthalpy=	0.138290
Thermal correction to Gibbs Free Energy=	0.088191
Sum of electronic and zero-point Energies=	-642.530375

Sum of electronic and thermal Energies= -642.519358
Sum of electronic and thermal Enthalpies= -642.518414
Sum of electronic and thermal Free Energies= -642.568513

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.186	39.373	105.442

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.172098	1.035926	0.000009
2	6	0	1.576703	1.087030	0.000021
3	7	0	2.178128	-0.172909	0.000017
4	6	0	1.488020	-1.343417	0.000001
5	6	0	0.114427	-1.322017	-0.000010
6	6	0	-0.583326	-0.095390	-0.000007
7	6	0	-0.484003	2.359803	0.000013
8	8	0	2.235401	2.112154	0.000035
9	1	0	3.193049	-0.181508	0.000025
10	8	0	2.294803	-2.418921	0.000000
11	1	0	-0.456565	-2.246321	-0.000023
12	6	0	-2.938565	-0.426831	-0.000026
13	8	0	-2.910323	-1.611234	-0.000036
14	8	0	-3.378892	0.672185	-0.000020
15	1	0	-0.180060	2.921878	0.887049
16	1	0	-0.180045	2.921892	-0.887008
17	1	0	-1.557690	2.186594	0.000003
18	1	0	1.762277	-3.232178	-0.000011

decarboxylation pathway for 1-methylorotate 4-protonated, isomer 2 (favored isomer) r = 2.65Å

SCF Done: E(RB+HF-LYP) = -642.657382864

Zero-point correction= 0.126157 (Hartree/Particle)
Thermal correction to Energy= 0.138261
Thermal correction to Enthalpy= 0.139205
Thermal correction to Gibbs Free Energy= 0.085467
Sum of electronic and zero-point Energies= -642.531226
Sum of electronic and thermal Energies= -642.519122
Sum of electronic and thermal Enthalpies= -642.518178
Sum of electronic and thermal Free Energies= -642.571916

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.760	41.574	113.101

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.263948	1.041628	0.000046
2	6	0	-1.667969	1.044259	-0.000034
3	7	0	-2.224943	-0.235244	-0.000057
4	6	0	-1.491200	-1.379377	0.000000
5	6	0	-0.120134	-1.307073	0.000084
6	6	0	0.546477	-0.056703	0.000106
7	6	0	0.339817	2.388912	0.000063
8	8	0	-2.364747	2.045517	-0.000080
9	1	0	-3.238644	-0.280608	-0.000119

10	8	0	-2.260572	-2.484648	-0.000038
11	1	0	0.473742	-2.217452	0.000137
12	6	0	3.177190	-0.375842	-0.000019
13	8	0	3.079749	-1.547372	0.000286
14	8	0	3.511207	0.750180	-0.000337
15	1	0	0.017825	2.941710	-0.886809
16	1	0	0.017831	2.941685	0.886954
17	1	0	1.419029	2.252431	0.000058
18	1	0	-1.697722	-3.276928	0.000009

decarboxylation pathway for 1-methylorotate 4-protonated, isomer 2 (favored isomer) pi complex with r = 2.913

SCF Done: E(RB+HF-LYP) = -642.657838372

Zero-point correction=	0.126076 (Hartree/Particle)
Thermal correction to Energy=	0.138287
Thermal correction to Enthalpy=	0.139231
Thermal correction to Gibbs Free Energy=	0.084765
Sum of electronic and zero-point Energies=	-642.531762
Sum of electronic and thermal Energies=	-642.519551
Sum of electronic and thermal Enthalpies=	-642.518607
Sum of electronic and thermal Free Energies=	-642.573074

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	86.776	41.606	114.634

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.344618	-1.043724	0.000432
2	6	0	-1.747804	-1.015263	-0.000176
3	7	0	-2.276172	0.276000	-0.000303
4	6	0	-1.515958	1.402985	0.000024
5	6	0	-0.147299	1.299012	0.000524
6	6	0	0.496347	0.033754	0.000747
7	6	0	0.226411	-2.404663	0.000623
8	8	0	-2.467905	-2.000591	-0.000564
9	1	0	-3.288475	0.344351	-0.000711
10	8	0	-2.261038	2.525960	-0.000214
11	1	0	0.462851	2.198894	0.000754
12	6	0	3.393619	0.337632	-0.000295
13	8	0	3.259113	1.501786	0.000131
14	8	0	3.660457	-0.802455	-0.000809
15	1	0	-0.108046	-2.951009	0.887037
16	1	0	-0.106233	-2.950525	-0.886780
17	1	0	1.308433	-2.290768	0.001741
18	1	0	-1.679912	3.304787	0.000035

potential energy saddle point for 1-methylorotate 4-protonated, isomer 2 + a hydrogen bonded water molecule

SCF Done: E(RB+HF-LYP) = -719.098336599

Zero-point correction=	0.150502 (Hartree/Particle)
Thermal correction to Energy=	0.165081
Thermal correction to Enthalpy=	0.166025
Thermal correction to Gibbs Free Energy=	0.106736

Sum of electronic and zero-point Energies= -718.947834
Sum of electronic and thermal Energies= -718.933256
Sum of electronic and thermal Enthalpies= -718.932312
Sum of electronic and thermal Free Energies= -718.991601

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	103.590	49.358	124.784

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.238972	-0.934021	-0.000022
2	6	0	-0.530230	-2.144186	0.000087
3	7	0	0.854402	-1.978874	0.000157
4	6	0	1.483964	-0.771076	0.000123
5	6	0	0.716779	0.376580	0.000013
6	6	0	-0.690697	0.317416	-0.000062
7	6	0	-2.706052	-1.088992	-0.000096
8	8	0	-1.043904	-3.252055	0.000121
9	1	0	1.404805	-2.831341	0.000237
10	8	0	2.811497	-0.870327	0.000204
11	1	0	1.198997	1.347921	-0.000013
12	6	0	-1.670640	2.660355	-0.000238
13	8	0	-0.617520	3.193305	-0.000207
14	8	0	-2.827149	2.437535	-0.000291
15	1	0	-3.022362	-1.645474	-0.886810
16	1	0	-3.022461	-1.645384	0.886639
17	1	0	-3.132775	-0.088199	-0.000171
18	1	0	3.233351	0.027147	0.000175
19	8	0	4.006290	1.591443	0.000141
20	1	0	3.889967	2.162903	-0.775409
21	1	0	3.890007	2.162907	0.775694

1-methyluracil carbene isomer 1 (disfavored isomer)

SCF Done: E(RB+HF-LYP) = -454.051777740
Zero-point correction= 0.112706 (Hartree/Particle)
Thermal correction to Energy= 0.120312
Thermal correction to Enthalpy= 0.121256
Thermal correction to Gibbs Free Energy= 0.080507
Sum of electronic and zero-point Energies= -453.939071
Sum of electronic and thermal Energies= -453.931466
Sum of electronic and thermal Enthalpies= -453.930522
Sum of electronic and thermal Free Energies= -453.971271

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	75.497	28.468	85.764

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.127539	-0.490128	-0.000206
2	6	0	-0.690174	0.838976	-0.000132
3	7	0	0.706031	0.957602	-0.000128
4	6	0	1.564609	-0.105661	0.000013
5	6	0	1.052880	-1.377701	0.000097
6	6	0	-0.346416	-1.618781	-0.000021
7	6	0	-2.593283	-0.683893	0.000037
8	8	0	-1.392866	1.839369	0.000170
9	1	0	1.029166	1.919216	-0.000057

10	8	0	2.890144	0.140412	0.000058
11	1	0	1.746409	-2.211736	0.000226
12	1	0	-2.869834	-1.251772	0.890587
13	1	0	-3.090863	0.285339	-0.003830
14	1	0	-2.868855	-1.258697	-0.886300
15	1	0	3.100614	1.089441	-0.000060

1-methyluracil carbene isomer 2 (favored isomer)

SCF Done: E(RB+HF-LYP) = -454.053457297

Zero-point correction=	0.112883 (Hartree/Particle)
Thermal correction to Energy=	0.121174
Thermal correction to Enthalpy=	0.122119
Thermal correction to Gibbs Free Energy=	0.079999
Sum of electronic and zero-point Energies=	-453.940575
Sum of electronic and thermal Energies=	-453.932283
Sum of electronic and thermal Enthalpies=	-453.931339
Sum of electronic and thermal Free Energies=	-453.973458

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	76.038	30.424	88.648

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.118895	-0.509810	-0.000188
2	6	0	-0.694685	0.821581	-0.000011
3	7	0	0.697815	0.962674	-0.000265
4	6	0	1.567333	-0.093112	-0.000024
5	6	0	1.069312	-1.369906	0.000170
6	6	0	-0.328480	-1.631677	0.000065
7	6	0	-2.585773	-0.666913	-0.000073
8	8	0	-1.425759	1.800929	0.000309
9	1	0	1.010404	1.927748	-0.000677
10	8	0	2.890709	0.167101	-0.000041
11	1	0	1.771839	-2.196273	0.000446
12	1	0	-3.015464	-0.193700	0.887654
13	1	0	-3.015713	-0.192659	-0.887112
14	1	0	-2.780130	-1.737515	-0.000656
15	1	0	3.090779	1.118270	0.000606

OROTATE anion

Becke3LYP/6-31+G*
SCF Done: E(RB+HF-LYP) = -602.909514492

Zero-point correction= (Hartree/Particle)	0.088543
Thermal correction to Energy=	0.097227
Thermal correction to Enthalpy=	0.098171
Thermal correction to Gibbs Free Energy=	0.053965
Sum of electronic and zero-point Energies=	-602.820971
Sum of electronic and thermal Energies=	-602.812287
Sum of electronic and thermal Enthalpies=	-602.811343
Sum of electronic and thermal Free Energies=	-602.855550

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	61.011	31.863	93.041

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.957379	0.108323	0.000000
2	6	-1.465391	-1.217688	0.000010
3	6	-0.022181	-1.303550	0.000000
4	6	0.730420	-0.169111	0.000000
5	7	0.132172	1.069420	0.000000
6	6	-1.223968	1.287282	-0.000010
7	1	-2.965279	0.213864	0.000000
8	8	-2.271503	-2.153177	0.000000
9	1	0.458117	-2.272741	0.000010
10	1	0.794173	1.847739	0.000000
11	8	-1.752046	2.399543	0.000000
12	6	2.287690	-0.102293	0.000010
13	8	2.728432	1.079626	-0.000010
14	8	2.876369	-1.201104	0.000000

DEPROTONATED URACIL (Uracil missing proton at C6 - vinylic anion product after decarboxylation of orotate)

Becke3LYP/6-31+G*
SCF Done: E(RB+HF-LYP) = -414.247753428

Zero-point correction= (Hartree/Particle)	0.073491
Thermal correction to Energy=	0.079519
Thermal correction to Enthalpy=	0.080463
Thermal correction to Gibbs Free Energy=	0.043199
Sum of electronic and zero-point Energies=	-414.174263
Sum of electronic and thermal Energies=	-414.168235
Sum of electronic and thermal Enthalpies=	-414.167291
Sum of electronic and thermal Free Energies=	-414.204554

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	49.899	22.563	78.428

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.000000	0.947620	0.000000
2	6	1.275730	0.325339	0.000000
3	6	1.213849	-1.110261	0.000000
4	6	0.042709	-1.858210	0.000000
5	7	-1.116061	-1.061780	0.000000
6	6	-1.222910	0.312720	0.000000
7	1	-0.014140	1.960860	0.000000
8	8	2.277630	1.065929	0.000000
9	1	2.177509	-1.615251	0.000000
10	1	-2.015131	-1.526090	0.000000
11	8	-2.301640	0.929331	0.000000

CARBON DIOXIDE

Becke3LYP/6-31+G*
SCF Done: E(RB+HF-LYP) = -188.587512597

Zero-point correction= (Hartree/Particle)	0.010722
Thermal correction to Energy=	0.013744
Thermal correction to Enthalpy=	0.014688
Thermal correction to Gibbs Free Energy=	-0.004979
Sum of electronic and zero-point Energies=	-188.576790
Sum of electronic and thermal Energies=	-188.573769
Sum of electronic and thermal Enthalpies=	-188.572825
Sum of electronic and thermal Free Energies=	-188.592492

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	8.624	7.159	41.394

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.143400
3	8	0.000287	0.000000	2.286800

OROTIC ACID

Becke3LYP/6-31+G*
SCF Done: E(RB+HF-LYP) = -603.416080542

Zero-point correction= (Hartree/Particle)	0.101699
Thermal correction to Energy=	0.110663
Thermal correction to Enthalpy=	0.111608
Thermal correction to Gibbs Free Energy=	0.066940
Sum of electronic and zero-point Energies=	-603.314382
Sum of electronic and thermal Energies=	-603.305417
Sum of electronic and thermal Enthalpies=	-603.304473
Sum of electronic and thermal Free Energies=	-603.349141

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	69.442	33.407	94.012

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.015786	0.018139	-0.000027
2	6	1.440386	-1.264516	-0.000052
3	6	-0.023421	-1.255931	-0.000012
4	6	-0.684912	-0.073835	-0.000022
5	7	-0.019245	1.131739	-0.000039
6	6	1.365334	1.246812	0.000000
7	1	3.030423	0.060000	0.000020
8	8	2.139550	-2.267023	0.000058
9	1	-0.542669	-2.203976	0.000014
10	1	-0.558548	1.991856	-0.000002
11	8	1.944709	2.318412	0.000043
12	6	-2.172901	0.067723	-0.000007
13	8	-2.727224	1.148748	0.000030
14	8	-2.816669	-1.111695	-0.000009

15	1	-3.774830	-0.926085	0.000017

4-PROTONATED 6-DEPROTONATED URACIL (Carbene)

Becke3LYP/6-31+G*
SCF Done: E(RB+HF-LYP) = -414.750760701

Zero-point correction= (Hartree/Particle)	0.086147
Thermal correction to Energy=	0.092451
Thermal correction to Enthalpy=	0.093395
Thermal correction to Gibbs Free Energy=	0.055750
Sum of electronic and zero-point Energies=	-414.664614
Sum of electronic and thermal Energies=	-414.658310
Sum of electronic and thermal Enthalpies=	-414.657366
Sum of electronic and thermal Free Energies=	-414.695011

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	58.014	24.084	79.231

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.031829	-0.939150	0.000010
2	6	-1.168979	-0.186771	0.000030
3	6	-1.095551	1.185079	0.000020
4	6	0.156059	1.866230	-0.000020
5	7	1.221369	1.008441	-0.000040
6	6	1.249611	-0.389129	-0.000010
7	1	-0.094198	-1.951850	0.000020
8	8	-2.279009	-0.951052	0.000060
9	1	-2.015721	1.764408	0.000040
10	1	2.155239	1.409212	-0.000080
11	8	2.260151	-1.070878	-0.000060
12	1	-3.068079	-0.383833	0.000090

2-PROTONATED 6-DEPROTONATED URACIL

Becke3LYP/6-31+G*
SCF Done: E(RB+HF-LYP) = -414.720822091

Zero-point correction= (Hartree/Particle)	0.084688
Thermal correction to Energy=	0.091393
Thermal correction to Enthalpy=	0.092337
Thermal correction to Gibbs Free Energy=	0.053858
Sum of electronic and zero-point Energies=	-414.636134
Sum of electronic and thermal Energies=	-414.629429
Sum of electronic and thermal Enthalpies=	-414.628485
Sum of electronic and thermal Free Energies=	-414.666964

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	57.350	25.081	80.987

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	7	0.000043	-0.935359	0.000000
2	6	-1.339598	-0.331357	-0.000015
3	6	-1.285178	1.103771	-0.000014
4	6	-0.145471	1.886732	-0.000001
5	7	1.051605	1.095389	0.000013
6	6	1.125557	-0.226037	0.000013
7	1	0.004337	-1.951054	-0.000001
8	8	-2.279465	-1.112451	-0.000027
9	1	-2.255244	1.592569	-0.000025
10	1	1.936200	1.592206	0.000023
11	8	2.343570	-0.786753	0.000026
12	1	2.308471	-1.758947	0.000025

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