Hydrolytic Stability of N-Methyl-2,6-Dimesityl-4,4'-Pyrylogen bis-Tetrafluoroborate

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Supporting Information

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Computational Details

N-Methyl-2,6-Dimesityl-4,4'-Pyrylogen Dication, 1^{2+} (Symmetrical-isomer)

C	0.009023	0.003221	0.008707	C	0.988451	-0.991053	-0.174646
C	2.158468	-0.958149	0.561553	C	1.460881	0.988830	1.674598
C	0.275677	1.004853	0.957884	C	-1.257956	-0.006560	-0.767724
C	-1.801439	1.194077	-1.248821	C	-2.983953	1.177715	-1.982579
C	-3.120727	-1.213681	-1.733396	C	-1.922491	-1.214874	-1.023541
H	0.861826	-1.782173	-0.904969	H	2.941970	-1.698001	0.442371
H	1.695532	1.737700	2.421548	H	-0.441931	1.789028	1.170618
H	-1.325189	2.145839	-1.060137	H	-1.525894	-2.160972	-0.683475
C	3.665031	0.022713	2.232561	H	3.813638	-0.959161	2.683711
H	4.484050	0.252263	1.547549	H	3.613447	0.779132	3.013481
C	-3.931281	-2.363354	-2.090451	C	-4.168916	-3.397617	-1.130585
C	-4.481210	-2.465985	-3.410270	C	-4.950695	-4.486110	-1.509575
C	-5.228779	-3.595791	-3.726898	C	-5.488826	-4.615119	-2.797880
H	-5.159385	-5.258283	-0.774346	H	-5.617437	-3.695081	-4.736441
C	-3.684900	2.319619	-2.541651	C	-2.954241	3.346708	-3.218613
C	-5.106630	2.422338	-2.398894	C	-3.659768	4.429598	-3.736617
C	-5.742024	3.546832	-2.917430	C	-5.049395	4.559407	-3.598088
H	-3.112504	5.196153	-4.278333	H	-6.815157	3.645801	-2.781166
N	2.383890	0.019385	1.473979	O	-3.587134	-0.021166	-2.181230
C	-1.459591	3.303545	-3.465088	H	-0.895757	3.738513	-2.629937
H	-1.081279	2.292889	-3.640350	H	-1.213281	3.899708	-4.346385
C	-5.950520	1.412070	-1.650750	H	-6.160135	0.526374	-2.258340
H	-5.476933	1.072078	-0.724432	H	-6.909712	1.858197	-1.381361
C	-5.777403	5.736194	-4.185854	H	-6.044184	5.530684	-5.230700
H	-6.704981	5.946518	-3.647745	H	-5.157055	6.636426	-4.181113
C	-4.233667	-1.450899	-4.506339	H	-4.872173	-0.568896	-4.396871
H	-3.195817	-1.104724	-4.533505	H	-4.454172	-1.895779	-5.478485
C	-3.673959	-3.358552	0.301142	H	-2.667294	-3.785462	0.396012
H	-3.656378	-2.350013	0.722802	H	-4.325882	-3.964203	0.934272
C	-6.341104	-5.796868	-3.167989	H	-7.401674	-5.559911	-3.012370
H	-6.221040	-6.063435	-4.221453	H	-6.108173	-6.671365	-2.555556

Zero-point correction= 0.524888 (Hartree/Particle)
Thermal correction to Energy= 0.555468
Thermal correction to Enthalpy= 0.556413
Thermal correction to Gibbs Free Energy= 0.460840
Sum of electronic and zero-point Energies= -1252.773657
Sum of electronic and thermal Energies= -1252.743077
Sum of electronic and thermal Enthalpies= -1252.742133
Sum of electronic and thermal Free Energies= -1252.837706

N-Methyl-2,6-Dimesityl-4,4'-Pyrylogen Dication, 1^{2+} (Anti-Isomer)

C	0.022857	-0.002412	0.002935	C	1.086627	0.847424	-0.347294
C	2.259876	0.834707	0.387184	C	1.398166	-0.814645	1.820002
C	0.208037	-0.844225	1.113852	C	-1.248088	-0.010222	-0.769735
C	-1.773766	1.187909	-1.275910	C	-2.967910	1.175957	-1.991567
C	-3.124094	-1.212203	-1.716359	C	-1.931846	-1.213726	-0.995371
H	1.025811	1.504262	-1.207287	H	3.105091	1.467167	0.142108
H	1.574460	-1.439251	2.687961	H	-0.575811	-1.510581	1.454778
H	-1.313036	2.141691	-1.060142	H	-1.518989	-2.163342	-0.685361
C	3.660052	0.053405	2.256250	H	4.487293	0.338181	1.607251
H	3.545738	0.783161	3.061163	H	3.847840	-0.936281	2.671099
C	-3.937978	-2.357984	-2.078036	C	-4.181909	-3.393215	-1.122265
C	-4.488968	-2.455027	-3.398855	C	-4.970411	-4.476989	-1.503288
C	-5.242525	-3.579356	-3.717689	C	-5.508061	-4.600508	-2.791247
H	-5.183913	-5.249176	-0.769698	H	-5.632247	-3.673842	-4.727458
C	-3.675579	2.315968	-2.545924	C	-2.953634	3.342830	-3.232456
C	-5.096457	2.415893	-2.394134	C	-3.665676	4.419174	-3.754283
C	-5.739198	3.534745	-2.916693	C	-5.055297	4.544344	-3.609542
H	-3.124263	5.185115	-4.302666	H	-6.811502	3.631477	-2.772640
N	2.405756	0.013922	1.454760	O	-3.580671	-0.020387	-2.175331
C	-1.459637	3.306828	-3.483136	H	-0.897467	3.741921	-2.646734
H	-1.079921	2.297283	-3.664432	H	-1.217448	3.907064	-4.362761
C	-5.933612	1.411650	-1.630179	H	-6.155823	0.524632	-2.231441
H	-5.448793	1.073690	-0.709182	H	-6.887013	1.863161	-1.349321
C	-5.790741	5.714177	-4.201879	H	-6.051160	5.505319	-5.247641
H	-6.722102	5.917603	-3.667787	H	-5.177811	6.619535	-4.195537
C	-4.234091	-1.440493	-4.493959	H	-4.863259	-0.552141	-4.382872
H	-3.192500	-1.105688	-4.522268	H	-4.460178	-1.882433	-5.466147
C	-3.687524	-3.362967	0.309769	H	-2.684806	-3.800318	0.400848
H	-3.663478	-2.355157	0.733666	H	-4.344839	-3.964863	0.940936
C	-6.356347	-5.781269	-3.173909	H	-7.405564	-5.479052	-3.280441
H	-6.044075	-6.194504	-4.138303	H	-6.310438	-6.574483	-2.424794

Zero-point correction= 0.524887 (Hartree/Particle)
Thermal correction to Energy= 0.555494
Thermal correction to Enthalpy= 0.556439
Thermal correction to Gibbs Free Energy= 0.459704
Sum of electronic and zero-point Energies= -1252.772913
Sum of electronic and thermal Energies= -1252.742306
Sum of electronic and thermal Enthalpies= -1252.741362
Sum of electronic and thermal Free Energies= -1252.838096

N-Methyl-2,6-Dimesityl-4,4'-Pyrylogen Dication, 1^{2+} (B3LYP/6-311+G(2d,p))

C	-0.002434	0.001460	-0.002198	C	0.975186	-0.985379	-0.189208
C	2.140724	-0.952156	0.542188	C	1.440871	0.978878	1.660299
C	0.260790	0.995199	0.947275	C	-1.267414	-0.007493	-0.776104
C	-1.808569	1.188487	-1.254107	C	-2.987935	1.174035	-1.980742
C	-3.124352	-1.207829	-1.735611	C	-1.930396	-1.209876	-1.030573
H	0.849784	-1.772821	-0.919984	H	2.923773	-1.688263	0.419279
H	1.673220	1.722851	2.409394	H	-0.456974	1.775046	1.162531
H	-1.332403	2.137456	-1.065641	H	-1.533737	-2.154287	-0.693989
C	3.640638	0.021338	2.215016	H	3.784020	-0.955969	2.671629
H	4.459740	0.241186	1.531657	H	3.590653	0.782651	2.987776
C	-3.929259	-2.357857	-2.090876	C	-4.167833	-3.384168	-1.132995
C	-4.471421	-2.467037	-3.408039	C	-4.944520	-4.470699	-1.508932
C	-5.211842	-3.593408	-3.721515	C	-5.472834	-4.605712	-2.792652
H	-5.157025	-5.236795	-0.772346	H	-5.595227	-3.697438	-4.730145
C	-3.685765	2.317089	-2.533176	C	-2.959273	3.333358	-3.218422
C	-5.098777	2.429892	-2.375114	C	-3.660910	4.411409	-3.734596
C	-5.730512	3.550171	-2.891007	C	-5.042383	4.549096	-3.583329
H	-3.116262	5.169984	-4.285114	H	-6.798560	3.657543	-2.741423
N	2.363624	0.017972	1.455154	O	-3.592185	-0.019568	-2.180157
C	-1.470539	3.281079	-3.476876	H	-0.899171	3.708108	-2.646465
H	-1.102717	2.270203	-3.656779	H	-1.228222	3.876615	-4.356175
C	-5.939217	1.433744	-1.610997	H	-6.179103	0.557344	-2.216289
H	-5.449400	1.082182	-0.700995	H	-6.880865	1.894823	-1.317027
C	-5.767225	5.724095	-4.169059	H	-6.033372	5.518862	-5.211415
H	-6.692103	5.934882	-3.632106	H	-5.146275	6.620691	-4.165168
C	-4.220816	-1.458543	-4.505008	H	-4.863980	-0.582098	-4.405714
H	-3.187032	-1.108051	-4.523805	H	-4.429528	-1.909297	-5.473930
C	-3.683663	-3.339075	0.298535	H	-2.682381	-3.769855	0.400840
H	-3.662967	-2.330426	0.712415	H	-4.341652	-3.936117	0.928776
C	-6.308065	-5.792320	-3.171212	H	-7.353101	-5.495178	-3.302987
H	-5.976980	-6.217182	-4.121293	H	-6.273989	-6.571660	-2.411060

Zero-point correction= 0.523239 (Hartree/Particle)
Thermal correction to Energy= 0.553779
Thermal correction to Enthalpy= 0.554723
Thermal correction to Gibbs Free Energy= 0.459149
Sum of electronic and zero-point Energies= -1253.039531
Sum of electronic and thermal Energies= -1253.008991
Sum of electronic and thermal Enthalpies= -1253.008047
Sum of electronic and thermal Free Energies= -1253.103621

N-Methyl-2,6-Dimesityl-4,4'-Pyrylogen Radical cation, $1^{+\bullet}$ (B3LYP/6-31+G(d,p))

C	-0.016091	-0.000598	-0.000197	C	0.609551	-1.199112	0.471749
C	1.779788	-1.166980	1.179564	C	1.849297	1.185679	1.043818
C	0.681467	1.205193	0.331961	C	-1.242424	-0.006909	-0.743998
C	-1.859717	1.193071	-1.218258	C	-3.020988	1.170819	-1.937992
C	-3.109746	-1.203365	-1.771021	C	-1.938729	-1.213968	-1.067492
H	0.177000	-2.172872	0.284132	H	2.261628	-2.068315	1.538338
H	2.383805	2.092337	1.300273	H	0.305080	2.174806	0.034127
H	-1.436697	2.166848	-1.014909	H	-1.559497	-2.183754	-0.776946
C	3.700286	0.018187	2.182782	H	3.759452	-0.853737	2.835016
H	4.526276	-0.007013	1.465347	H	3.776315	0.919142	2.793085
C	-3.908345	-2.383059	-2.160178	C	-4.424191	-3.251688	-1.169266
C	-4.146522	-2.638210	-3.535262	C	-5.171096	-4.362374	-1.578111
C	-4.887038	-3.767948	-3.885900	C	-5.414543	-4.641769	-2.926070
H	-5.579557	-5.023892	-0.818249	H	-5.053244	-3.975992	-4.940110
C	-3.742580	2.342377	-2.473489	C	-3.097072	3.228978	-3.368915
C	-5.085118	2.573045	-2.076736	C	-3.812971	4.330808	-3.849819
C	-5.746194	3.695391	-2.578009	C	-5.134195	4.585394	-3.469957
H	-3.324122	5.005538	-4.548190	H	-6.768440	3.884130	-2.259290
N	2.409246	0.012830	1.479316	O	-3.638645	-0.019692	-2.205543
C	-1.673732	3.028100	-3.848045	H	-0.941362	3.412238	-3.127248
H	-1.436056	1.975398	-4.025042	H	-1.511563	3.568987	-4.783598
C	-5.809091	1.664927	-1.106468	H	-6.125560	0.733271	-1.586689
H	-5.180794	1.394451	-0.250773	H	-6.702489	2.159428	-0.718164
C	-5.890578	5.769149	-4.020875	H	-6.540984	5.462495	-4.849243
H	-6.529920	6.223829	-3.257968	H	-5.212208	6.537444	-4.401492
C	-3.596952	-1.746947	-4.627878	H	-4.166799	-0.815832	-4.713232
H	-2.551337	-1.474535	-4.446918	H	-3.644221	-2.255519	-5.593614
C	-4.221368	-3.023072	0.314712	H	-3.254017	-3.409400	0.658864
H	-4.264599	-1.964338	0.585074	H	-4.993039	-3.545343	0.885647
C	-6.239577	-5.835520	-3.340213	H	-7.258417	-5.529550	-3.607497
H	-5.810185	-6.331523	-4.216262	H	-6.315554	-6.570018	-2.534158

Zero-point correction= 0.522814 (Hartree/Particle)
Thermal correction to Energy= 0.554141
Thermal correction to Enthalpy= 0.555085
Thermal correction to Gibbs Free Energy= 0.454918
Sum of electronic and zero-point Energies= -1253.090384
Sum of electronic and thermal Energies= -1253.059058
Sum of electronic and thermal Enthalpies= -1253.058114
Sum of electronic and thermal Free Energies= -1253.158281

Neutral N-Methyl-2,6-Dimesityl-4,4'-Pyrylogen, 1^0 (B3LYP/6-31+G(d,p))

C	0.013898	0.004239	0.058289	C	0.668852	-1.202415	0.551729
C	1.812540	-1.164250	1.277973	C	1.877040	1.202071	1.145359
C	0.735591	1.220906	0.414954	C	-1.165002	-0.003929	-0.670569
C	-1.815110	1.199601	-1.170950	C	-2.961628	1.171913	-1.882331
C	-3.041198	-1.204201	-1.728126	C	-1.890662	-1.216603	-1.022374
H	0.247267	-2.179669	0.350770	H	2.294051	-2.066014	1.640023
H	2.406633	2.111357	1.407856	H	0.365174	2.191250	0.107796
H	-1.392428	2.177882	-0.977482	H	-1.517704	-2.189792	-0.727754
C	3.782828	0.020895	2.175173	H	3.905078	-0.835309	2.843880
H	4.549874	-0.036325	1.388234	H	3.947599	0.932031	2.756654
C	-3.828734	-2.394224	-2.140000	C	-4.435229	-3.227878	-1.175503
C	-3.976463	-2.687985	-3.518587	C	-5.167908	-4.343886	-1.606861
C	-4.713299	-3.811624	-3.899236	C	-5.320211	-4.654764	-2.959229
H	-5.638679	-4.979938	-0.860207	H	-4.812385	-4.038215	-4.959169
C	-3.690633	2.352520	-2.412994	C	-3.112089	3.169263	-3.408272
C	-4.983139	2.654111	-1.916781	C	-3.830424	4.278926	-3.878278
C	-5.658718	3.770996	-2.413679	C	-5.101153	4.598861	-3.396821
H	-3.383302	4.902176	-4.649909	H	-6.645960	4.004442	-2.019370
N	2.435466	0.026287	1.630917	O	-3.612529	-0.019924	-2.178784
C	-1.745141	2.885233	-3.995134	H	-0.938832	3.228270	-3.336332
H	-1.585485	1.815875	-4.158582	H	-1.627318	3.402252	-4.952021
C	-5.633264	1.803302	-0.849315	H	-5.944651	0.833098	-1.249860
H	-4.940729	1.600370	-0.024970	H	-6.515128	2.303818	-0.439775
C	-5.863511	5.793582	-3.922170	H	-6.779364	5.483960	-4.440002
H	-6.164197	6.463497	-3.108178	H	-5.260934	6.372591	-4.628025
C	-3.336070	-1.822970	-4.580678	H	-3.862308	-0.868719	-4.687209
H	-2.296295	-1.587207	-4.328839	H	-3.346959	-2.329557	-5.549894
C	-4.331174	-2.957304	0.310969	H	-3.377298	-3.307301	0.723152
H	-4.400010	-1.890059	0.538119	H	-5.129118	-3.477418	0.849252
C	-6.119656	-5.857545	-3.404977	H	-6.989600	-5.557570	-4.001464
H	-5.516398	-6.527505	-4.028822	H	-6.484253	-6.433699	-2.549548

Zero-point correction= 0.520492 (Hartree/Particle)
Thermal correction to Energy= 0.552039
Thermal correction to Enthalpy= 0.552983
Thermal correction to Gibbs Free Energy= 0.454523
Sum of electronic and zero-point Energies= -1253.274846
Sum of electronic and thermal Energies= -1253.243299
Sum of electronic and thermal Enthalpies= -1253.242355
Sum of electronic and thermal Free Energies= -1253.340815

E-3-(4-methylpyridinium)-1,5-diphenyl-2-pentene-1,5-dione (B3LYP/6-31G(d); Rotomer 1)

C	-2.167223	0.410657	-0.334769	C	-0.825487	0.571865	-0.262015
C	-0.074049	1.866852	-0.133753	C	-4.289995	1.313275	0.677202
C	-3.174260	1.537377	-0.353145	C	-2.688581	-0.973213	-0.444364
C	-3.724342	-1.307099	-1.342706	C	-4.157768	-2.607337	-1.462586
C	-2.608626	-3.318880	0.152860	C	-2.134340	-2.034951	0.300014
H	-0.210102	-0.321602	-0.289618	H	-2.652508	2.475939	-0.163612
H	-4.196370	-0.550271	-1.957682	H	-4.948395	-2.898176	-2.144025
H	-2.221935	-4.152412	0.727077	H	-1.357151	-1.848079	1.031387
O	-0.656313	2.916373	0.127694	C	-5.247318	2.413583	0.945568
C	-5.163665	3.664033	0.308418	C	-6.277955	2.181670	1.874788
C	-6.095947	4.659196	0.593117	H	-4.372993	3.871874	-0.405434
C	-7.204874	3.177831	2.158085	H	-6.329208	1.214172	2.362867
C	-7.115497	4.417778	1.516794	H	-6.024677	5.623542	0.099260
H	-7.996569	2.993512	2.878236	H	-7.839119	5.196705	1.739715
C	1.407521	1.833874	-0.286229	C	2.106110	0.762763	-0.871527
C	2.127925	2.958650	0.156364	C	3.491944	0.815583	-1.006108
H	1.578275	-0.104143	-1.257077	C	3.511650	3.002402	0.033903
H	1.579354	3.784460	0.596356	C	4.196729	1.930313	-0.547259
H	4.021773	-0.010908	-1.470310	H	4.059369	3.870665	0.387860
H	5.277956	1.965638	-0.645284	N	-3.608564	-3.602825	-0.719910
C	-4.143583	-4.978549	-0.815053	H	-3.349795	-5.688504	-0.581549
H	-4.969668	-5.100441	-0.109546	H	-4.495754	-5.156284	-1.831653
O	-4.374684	0.226447	1.242490	H	-3.635181	1.633800	-1.348782

Zero-point correction= 0.374679 (Hartree/Particle)
Thermal correction to Energy= 0.397307
Thermal correction to Enthalpy= 0.398251
Thermal correction to Gibbs Free Energy= 0.318317
Sum of electronic and zero-point Energies= -1093.091272
Sum of electronic and thermal Energies= -1093.068643
Sum of electronic and thermal Enthalpies= -1093.067699
Sum of electronic and thermal Free Energies= -1093.147633

E-3-(4-methylpyridinium)-1,5-diphenyl-2-pentene-1,5-dione (B3LYP/6-31G(d); Rotomer 2)

C	-1.856552	0.478919	0.444224	C	-0.519517	0.534542	0.233059
C	0.396431	1.669725	0.588740	C	-3.212753	2.600941	-0.079271
C	-2.684128	1.625872	1.002159	C	-2.555697	-0.780012	0.092394
C	-3.841150	-0.776930	-0.487533	C	-4.465219	-1.965653	-0.801518
C	-2.645139	-3.200721	0.021895	C	-1.975021	-2.040218	0.346541
H	-0.035771	-0.327407	-0.217518	H	-3.578114	1.227579	1.499139

H	-4.308792	0.170795	-0.741296	H	-5.443530	-2.003325	-1.266282
H	-2.234701	-4.184971	0.214026	H	-1.006280	-2.120301	0.825840
O	0.093483	2.450225	1.488371	C	-3.099106	4.066576	0.114319
C	-2.293505	4.664479	1.099958	C	-3.851418	4.887611	-0.750146
C	-2.250176	6.052585	1.218588	H	-1.668454	4.064447	1.750716
C	-3.809687	6.269761	-0.621984	H	-4.465329	4.416149	-1.509825
C	-3.009402	6.855097	0.365421	H	-1.619446	6.507225	1.976569
H	-4.398052	6.894268	-1.287721	H	-2.976047	7.936328	0.465902
C	1.694149	1.777514	-0.127122	C	1.966733	1.088569	-1.322035
C	2.670244	2.637440	0.408158	C	3.191768	1.254137	-1.964486
H	1.217615	0.445658	-1.774826	C	3.896457	2.790228	-0.227944
H	2.444901	3.171586	1.325030	C	4.159299	2.098468	-1.415235
H	3.391513	0.727919	-2.893129	H	4.648781	3.448577	0.196008
H	5.116815	2.220392	-1.913481	N	-3.875207	-3.161668	-0.548180
C	-4.595304	-4.420850	-0.843103	H	-3.871046	-5.200384	-1.080586
H	-5.187995	-4.716290	0.026553	H	-5.249551	-4.264833	-1.701140
O	-3.782438	2.131556	-1.061215	H	-2.091683	2.133635	1.757160

Zero-point correction= 0.375207 (Hartree/Particle)
Thermal correction to Energy= 0.397640
Thermal correction to Enthalpy= 0.398584
Thermal correction to Gibbs Free Energy= 0.319268
Sum of electronic and zero-point Energies= -1093.090809
Sum of electronic and thermal Energies= -1093.068377
Sum of electronic and thermal Enthalpies= -1093.067433
Sum of electronic and thermal Free Energies= -1093.146749

Z-3-(4-methylpyridinium)-1,5-diphenyl-2-pentene-1,5-dione (B3LYP/6-31G(d))

C	-1.318782	0.195826	0.359354	C	-0.055125	-0.112463	0.701003
C	0.362446	-1.499054	1.061308	C	-2.573230	2.320017	0.992918
C	-1.706131	1.597966	-0.059029	C	-2.409945	-0.825456	0.345204
C	-2.849800	-1.384205	-0.865694	C	-3.893686	-2.287070	-0.876100
C	-4.149462	-2.074839	1.451224	C	-3.114035	-1.172117	1.514829
H	0.688942	0.676329	0.679808	H	-0.802382	2.187807	-0.246524
H	-2.359097	-1.143690	-1.802164	H	-4.246623	-2.760120	-1.784450
H	-4.709642	-2.385257	2.325359	H	-2.848534	-0.725147	2.462994
O	-0.448351	-2.418476	0.920849	C	-2.960208	3.731952	0.743277
C	-2.602900	4.424779	-0.426503	C	-3.716133	4.391468	1.729181
C	-2.995961	5.749143	-0.605860	H	-2.019009	3.940599	-1.203424
C	-4.104900	5.713935	1.548287	H	-3.983527	3.847334	2.628754
C	-3.745712	6.394393	0.380442	H	-2.716642	6.278386	-1.511913
H	-4.685953	6.217866	2.314897	H	-4.048937	7.427936	0.239789
C	1.737507	-1.750239	1.559482	C	2.623942	-0.722632	1.929469
C	2.153654	-3.089444	1.679941	C	3.896545	-1.030086	2.405410
H	2.326408	0.319170	1.872936	C	3.426988	-3.392444	2.145926
H	1.460342	-3.874424	1.397663	C	4.301273	-2.362503	2.509428

H	4.571871	-0.230905	2.695583	H	3.742369	-4.428304	2.228346
H	5.296449	-2.599020	2.874956	N	-4.528554	-2.630379	0.268831
C	-5.619173	-3.629523	0.257009	H	-6.466179	-3.245528	0.828262
H	-5.929903	-3.808902	-0.771798	H	-5.262318	-4.562289	0.700458
O	-2.919167	1.720793	2.003061	H	-2.261353	1.576735	-1.008071

Zero-point correction= 0.374382 (Hartree/Particle)
Thermal correction to Energy= 0.397161
Thermal correction to Enthalpy= 0.398106
Thermal correction to Gibbs Free Energy= 0.317150
Sum of electronic and zero-point Energies= -1093.094841
Sum of electronic and thermal Energies= -1093.072062
Sum of electronic and thermal Enthalpies= -1093.071117
Sum of electronic and thermal Free Energies= -1093.152073

2-hydroxy-2,6-dimesityl-4-(N-methylpyridinium)-2H-pyran, B3LYP/6-31G(d)

C	-0.181439	0.006232	0.058097	C	0.796193	-1.008927	-0.040056
C	1.925123	-0.979418	0.748207	C	1.205026	1.003704	1.779856
C	0.064052	1.019727	1.012136	C	-1.374640	0.001997	-0.794954
C	-1.934805	1.180474	-1.180802	C	-3.050484	1.195636	-2.192800
C	-3.137266	-1.225266	-1.905970	C	-1.938481	-1.244007	-1.272931
H	0.690650	-1.812088	-0.759137	H	2.697752	-1.736509	0.685792
H	1.416578	1.760487	2.526091	H	-0.654765	1.814427	1.172667
H	-1.549015	2.142200	-0.867330	H	-1.484245	-2.198210	-1.042202
C	3.319649	-0.000052	2.526531	H	3.059373	-0.437821	3.493867
H	4.104054	-0.591386	2.054185	H	3.675787	1.021587	2.665318
C	-3.909919	-2.423735	-2.314498	C	-4.343466	-3.360511	-1.348917
C	-4.212115	-2.620961	-3.683367	C	-5.066549	-4.478760	-1.775832
C	-4.924956	-3.760882	-4.056979	C	-5.367730	-4.701396	-3.121212
H	-5.408818	-5.194525	-1.031698	H	-5.138866	-3.920591	-5.111697
C	-4.046290	2.348031	-1.945673	C	-3.639905	3.670333	-2.283002
C	-5.331129	2.148968	-1.367116	C	-4.553062	4.721613	-2.145673
C	-6.191773	3.247022	-1.252045	C	-5.843428	4.535684	-1.655400
H	-4.232513	5.722822	-2.425126	H	-7.177122	3.081774	-0.822824
N	2.129093	0.014598	1.649323	O	-3.775353	-0.053820	-2.169816
C	-2.238060	4.079551	-2.713337	H	-1.621333	4.309798	-1.831799
H	-1.712882	3.324003	-3.293398	H	-2.283210	5.000254	-3.302544
C	-5.870692	0.840677	-0.812547	H	-6.122346	0.122330	-1.596727
H	-5.159195	0.347914	-0.143941	H	-6.779155	1.042644	-0.237677
C	-6.823363	5.678847	-1.560899	H	-7.454264	5.728071	-2.458036
H	-7.492110	5.564476	-0.701491	H	-6.310691	6.641726	-1.470278
C	-3.770891	-1.647374	-4.754047	H	-4.460419	-0.796599	-4.821392
H	-2.774670	-1.239392	-4.560182	H	-3.756753	-2.136385	-5.732453
C	-4.075808	-3.199869	0.133628	H	-3.069525	-3.540730	0.409628
H	-4.165220	-2.159937	0.462324	H	-4.785546	-3.798110	0.712527
C	-6.167966	-5.906309	-3.553086	H	-7.222552	-5.642701	-3.706662

H	-5.797093	-6.315045	-4.499110	H	-6.135030	-6.701181	-2.801688
O	-2.432379	1.272871	-3.461444	H	-3.120097	1.522208	-4.105083

Zero-point correction= 0.542035 (Hartree/Particle)
Thermal correction to Energy= 0.574127
Thermal correction to Enthalpy= 0.575071
Thermal correction to Gibbs Free Energy= 0.475804
Sum of electronic and zero-point Energies= -1328.794636
Sum of electronic and thermal Energies= -1328.762544
Sum of electronic and thermal Enthalpies= -1328.761600
Sum of electronic and thermal Free Energies= -1328.860868

4-hydroxy-2,6-dimesityl-4-(N-methylpyridinium)-4H-pyran, B3LYP/6-31G(d)

C	-0.303274	-0.158515	0.263030	C	0.446092	0.169165	1.403141
C	1.826105	0.191452	1.341205	C	1.779084	-0.425368	-0.926760
C	0.401300	-0.455722	-0.914473	C	-1.832359	-0.157327	0.280333
C	-2.331926	1.090902	-0.401209	C	-3.218515	1.078992	-1.415354
C	-3.320933	-1.293123	-1.393862	C	-2.405294	-1.364825	-0.410211
H	-0.056736	0.389777	2.335675	H	2.445131	0.435329	2.196482
H	2.364891	-0.654255	-1.809280	H	-0.132348	-0.723229	-1.819628
H	-1.999302	2.045083	-0.006962	H	-2.124042	-2.340687	-0.028985
C	3.958144	-0.045129	0.133148	H	4.268035	0.893023	-0.333982
H	4.358288	-0.102197	1.145069	H	4.328191	-0.890672	-0.448390
C	-3.995440	-2.450528	-2.035090	C	-4.869656	-3.268254	-1.287333
C	-3.760574	-2.718479	-3.403080	C	-5.485075	-4.349482	-1.926803
C	-4.392901	-3.813939	-3.992177	C	-5.263159	-4.641584	-3.274442
H	-6.163016	-4.977832	-1.353728	H	-4.201430	-4.027719	-5.041533
C	-3.788982	2.281240	-2.073162	C	-2.965116	3.142111	-2.827954
C	-5.170749	2.550732	-1.936313	C	-3.541761	4.265275	-3.429849
C	-5.695739	3.688667	-2.549140	C	-4.901375	4.558809	-3.304373
H	-2.909745	4.926389	-4.018490	H	-6.755664	3.903895	-2.432671
N	2.480014	-0.104134	0.191735	O	-3.719752	-0.090523	-1.933296
C	-1.484854	2.887843	-3.022671	H	-0.900971	3.149523	-2.131105
H	-1.276828	1.836298	-3.249096	H	-1.100900	3.490955	-3.850511
C	-6.079964	1.648585	-1.132267	H	-6.252400	0.694555	-1.642672
H	-5.653287	1.417499	-0.148331	H	-7.051509	2.123191	-0.970241
C	-5.506477	5.765369	-3.980327	H	-6.053907	5.474718	-4.886239
H	-6.219397	6.275371	-3.323428	H	-4.739644	6.487519	-4.276446
C	-2.836242	-1.857879	-4.235440	H	-3.277645	-0.876945	-4.443127
H	-1.880186	-1.679811	-3.725844	H	-2.617415	-2.337951	-5.193296
C	-5.178358	-3.010604	0.172786	H	-4.351066	-3.305562	0.829631
H	-5.383587	-1.952319	0.367957	H	-6.057742	-3.582281	0.482285
C	-5.961133	-5.798928	-3.947187	H	-6.855702	-5.458422	-4.484730
H	-5.310520	-6.287525	-4.680160	H	-6.282512	-6.551505	-3.220700
O	-2.161165	-0.153720	1.683170	H	-3.127022	-0.075339	1.742026

Zero-point correction= 0.541283 (Hartree/Particle)

Thermal correction to Energy= 0.573837
Thermal correction to Enthalpy= 0.574781
Thermal correction to Gibbs Free Energy= 0.473401
Sum of electronic and zero-point Energies= -1328.801885
Sum of electronic and thermal Energies= -1328.769331
Sum of electronic and thermal Enthalpies= -1328.768387
Sum of electronic and thermal Free Energies= -1328.869767

E-1,5-Dimesityl-3-(4-methylpyridinium)-2-penten-1,5-dione, 3E, (B3LYP/6-31G(d); Rotomer 1)

C	-1.255518	0.944116	0.569654	C	0.036828	0.724819	0.219945
C	1.197028	1.658009	0.457238	C	-2.004831	3.288125	-0.043471
C	-1.754518	2.265526	1.099599	C	-2.250411	-0.100772	0.290278
C	-3.600778	0.222135	0.021619	C	-4.521717	-0.763225	-0.259158
C	-2.887168	-2.426600	0.004601	C	-1.930338	-1.478939	0.284152
H	0.302695	-0.213633	-0.257591	H	-2.657079	2.142975	1.704986
H	-3.937865	1.251841	0.008171	H	-5.557872	-0.541658	-0.485775
H	-2.671638	-3.488616	0.000987	H	-0.929752	-1.817682	0.524330
O	1.112614	2.517704	1.330420	C	-3.054633	4.335796	0.143589
C	-3.189487	5.065084	1.353875	C	-3.926860	4.602957	-0.945701
C	-4.205824	6.016722	1.453721	C	-4.946113	5.543283	-0.773493
C	-5.104156	6.265134	0.411449	H	-4.293250	6.590607	2.373518
H	-5.627793	5.729196	-1.600293	C	2.455093	1.401048	-0.295010
C	2.435598	1.083863	-1.677136	C	3.694764	1.499857	0.396258
C	3.647853	0.849477	-2.330037	C	4.869696	1.221882	-0.302087
C	4.874221	0.899789	-1.663592	H	3.633442	0.631760	-3.395782
H	5.815840	1.268648	0.232249	N	-4.170376	-2.073366	-0.270632
C	-5.185518	-3.119678	-0.521927	H	-4.729168	-3.933646	-1.086518
H	-5.569312	-3.496349	0.429857	H	-6.001302	-2.692674	-1.105290
O	-1.388833	3.165698	-1.089939	H	-0.974892	2.677506	1.742843
C	-2.241843	4.923915	2.529591	H	-1.193090	4.880817	2.218404
H	-2.346248	5.784224	3.196188	H	-2.447210	4.030438	3.131606
C	-3.816488	3.920325	-2.293164	H	-2.965330	4.307852	-2.861177
H	-3.659666	2.839122	-2.215541	H	-4.725536	4.093554	-2.876747
C	-6.182138	7.311264	0.550934	H	-5.784002	8.311089	0.334154
H	-7.009170	7.131860	-0.142873	H	-6.586167	7.338420	1.568293
C	3.804054	1.870715	1.858873	H	3.608622	2.936492	2.011335
H	3.084759	1.333769	2.485303	H	4.810067	1.649474	2.226732
C	1.169195	1.044500	-2.512820	H	0.720992	0.040672	-2.530414
H	0.405463	1.747901	-2.171819	H	1.406158	1.293463	-3.551971
C	6.170352	0.652702	-2.394646	H	6.877334	0.090005	-1.775862
H	6.009542	0.097493	-3.323704	H	6.656146	1.601411	-2.657634

Zero-point correction= 0.541709 (Hartree/Particle)
Thermal correction to Energy= 0.574278
Thermal correction to Enthalpy= 0.575223

Thermal correction to Gibbs Free Energy= 0.473724
Sum of electronic and zero-point Energies= -1328.811412
Sum of electronic and thermal Energies= -1328.778842
Sum of electronic and thermal Enthalpies= -1328.777898
Sum of electronic and thermal Free Energies= -1328.879396

E-1,5-Dimesityl-3-(4-methylpyridinium)-2-penten-1,5-dione, 3E, (B3LYP/6-31G(d); Rotomer 2)

C	-2.303886	0.304561	-0.653733	C	-0.981466	0.555894	-0.504405
C	-0.301578	1.897744	-0.438883	C	-4.460615	1.221664	0.234922
C	-3.371906	1.355095	-0.854615	C	-2.735491	-1.113910	-0.651771
C	-3.666116	-1.613502	-1.589167	C	-4.002340	-2.946542	-1.604060
C	-2.554289	-3.377776	0.193673	C	-2.177901	-2.054725	0.239754
H	-0.311858	-0.292360	-0.396774	H	-2.918692	2.344209	-0.845201
H	-4.132155	-0.959973	-2.316533	H	-4.711015	-3.361708	-2.310836
H	-2.163164	-4.118649	0.880792	H	-1.475987	-1.740529	1.002860
O	-0.951020	2.937800	-0.400659	C	-5.238878	2.410625	0.672796
C	-5.678843	3.412711	-0.233695	C	-5.548941	2.529309	2.058174
C	-6.395420	4.502940	0.261874	C	-6.240125	3.660092	2.495980
C	-6.672439	4.660509	1.622230	H	-6.751436	5.253969	-0.439090
H	-6.454790	3.758383	3.557466	C	1.187207	1.890614	-0.308556
C	2.000411	1.121009	-1.174283	C	1.782315	2.705595	0.691357
C	3.387145	1.158916	-1.007872	C	3.169654	2.677899	0.833325
C	3.993234	1.913265	-0.000795	H	4.012610	0.592526	-1.694494
H	3.625397	3.284606	1.612571	N	-3.456221	-3.820887	-0.718455
C	-3.894077	-5.233010	-0.710304	H	-3.099169	-5.851910	-0.293675
H	-4.797981	-5.334262	-0.103812	H	-4.097009	-5.551495	-1.733507
O	-4.596083	0.121771	0.766155	H	-3.844870	1.223183	-1.837241
C	0.978415	3.593318	1.616166	H	0.606417	4.476934	1.088518
H	0.100113	3.085930	2.028011	H	1.599778	3.928787	2.451386
C	1.450834	0.302862	-2.328502	H	1.233617	-0.733992	-2.036770
H	0.536908	0.726695	-2.754740	H	2.189861	0.251078	-3.133843
C	5.490124	1.907518	0.187049	H	5.774650	1.286542	1.046494
H	6.004760	1.509401	-0.692515	H	5.872197	2.915891	0.379179
C	-5.479988	3.347514	-1.735515	H	-4.449025	3.571018	-2.032270
H	-5.745005	2.368617	-2.151057	H	-6.118830	4.085942	-2.226973
C	-5.150495	1.507101	3.100928	H	-5.758540	0.600834	3.022947
H	-4.107784	1.190347	3.001401	H	-5.285173	1.926245	4.102172
C	-7.400904	5.877792	2.133476	H	-8.027490	5.636425	2.998081
H	-6.689020	6.650026	2.453523	H	-8.036711	6.320507	1.360633

Zero-point correction= 0.541160 (Hartree/Particle)
Thermal correction to Energy= 0.574013
Thermal correction to Enthalpy= 0.574957
Thermal correction to Gibbs Free Energy= 0.471922
Sum of electronic and zero-point Energies= -1328.812947

Sum of electronic and thermal Energies= -1328.780094
Sum of electronic and thermal Enthalpies= -1328.779150
Sum of electronic and thermal Free Energies= -1328.882185

Z-1,5-Dimesityl-3-(4-methylpyridinium)-2-penten-1,5-dione, 3Z, (B3LYP/6-31G(d))

C	-1.593104	0.000349	0.227199	C	-0.334546	-0.197578	0.662306
C	0.152205	-1.514295	1.177604	C	-2.950505	2.125669	0.532361
C	-2.011322	1.316238	-0.397881	C	-2.634650	-1.067188	0.296180
C	-3.068313	-1.714748	-0.871323	C	-4.067133	-2.666491	-0.811296
C	-4.288486	-2.339521	1.506106	C	-3.298166	-1.388467	1.497392
H	0.380726	0.613809	0.575364	H	-1.127255	1.908066	-0.649960
H	-2.608921	-1.503056	-1.830350	H	-4.412622	-3.204074	-1.686010
H	-4.817986	-2.626965	2.406641	H	-3.036869	-0.885391	2.418224
O	-0.588011	-2.495129	1.072311	C	-2.966447	3.613942	0.450920
C	-2.957584	4.309980	-0.786306	C	-3.001886	4.343485	1.671474
C	-2.968217	5.705542	-0.774489	C	-2.976924	5.738616	1.618842
C	-2.959025	6.442974	0.412851	H	-2.990940	6.235385	-1.723907
H	-2.982514	6.293863	2.553823	C	1.538525	-1.616227	1.708895
C	2.073453	-0.634630	2.580096	C	2.327708	-2.739448	1.334332
C	3.385174	-0.782626	3.037792	C	3.640972	-2.815593	1.795606
C	4.192457	-1.853479	2.649542	H	3.785509	-0.040598	3.724966
H	4.253631	-3.659012	1.485312	N	-4.663921	-2.976161	0.361704
C	-5.716314	-4.012303	0.427571	H	-6.603084	-3.597331	0.910836
H	-5.970874	-4.329557	-0.583155	H	-5.347722	-4.868767	0.997082
O	-3.600008	1.509805	1.368225	H	-2.542821	1.126162	-1.339213
C	-3.010760	3.627512	-2.139798	H	-2.049110	3.185635	-2.427476
H	-3.768847	2.837087	-2.179277	H	-3.267128	4.355352	-2.914097
C	-2.917743	7.950490	0.392072	H	-1.880893	8.311644	0.403937
H	-3.392021	8.352912	-0.508482	H	-3.420434	8.377634	1.265435
C	-3.045955	3.690861	3.036577	H	-4.035935	3.273991	3.245085
H	-2.334862	2.864142	3.131220	H	-2.814736	4.428320	3.810455
C	1.283828	0.551649	3.101376	H	1.394718	1.435236	2.458911
H	0.214362	0.345482	3.199383	H	1.652298	0.837458	4.091241
C	1.819415	-3.846495	0.436694	H	1.109748	-4.490159	0.965320
H	1.294945	-3.464009	-0.444750	H	2.654295	-4.464358	0.093931
C	5.606577	-1.991708	3.155814	H	5.957331	-1.069763	3.628591
H	5.679227	-2.795558	3.899530	H	6.297037	-2.243305	2.343185

Zero-point correction= 0.540934 (Hartree/Particle)
Thermal correction to Energy= 0.573853
Thermal correction to Enthalpy= 0.574797
Thermal correction to Gibbs Free Energy= 0.471235
Sum of electronic and zero-point Energies= -1328.816030
Sum of electronic and thermal Energies= -1328.783112
Sum of electronic and thermal Enthalpies= -1328.782168
Sum of electronic and thermal Free Energies= -1328.885729

N-Methyl-2,6-Diphenyl-4,4'-Pyrylogen, 2^{2+}, (B3LYP/6-31+G(d,p))

C	-2.122171	0.586981	0.472760	C	-0.779254	0.578905	0.874008
C	0.023076	1.689509	0.622044	C	-1.813756	2.797181	-0.454109
C	-2.641005	1.707990	-0.189700	C	-2.992390	-0.588566	0.749152
C	-2.525864	-1.900473	0.561004	C	-3.355669	-2.977586	0.825849
C	-5.096320	-1.537149	1.468716	C	-4.310343	-0.427051	1.211174
H	-0.351546	-0.272096	1.386179	H	-3.673258	1.743351	-0.510209
H	-1.528118	-2.099090	0.186088	H	-3.037368	-4.003578	0.682945
H	-6.112562	-1.456696	1.837091	H	-4.727086	0.555199	1.403501
O	-0.528488	2.739007	-0.032052	C	-2.174923	4.027018	-1.125427
C	-3.353273	4.094329	-1.907238	C	-1.359247	5.176958	-1.003520
C	-3.699986	5.277254	-2.546521	H	-3.978813	3.219258	-2.047786
C	-1.720682	6.357501	-1.639952	H	-0.465117	5.147081	-0.391962
C	-2.888223	6.411201	-2.412354	H	-4.595994	5.318745	-3.156610
H	-1.099219	7.240154	-1.532317	H	-3.165109	7.335312	-2.909933
C	1.419125	1.855744	0.963915	C	2.026146	1.008316	1.921967
C	2.194931	2.861239	0.339546	C	3.367825	1.166657	2.242900
H	1.447992	0.252010	2.441964	C	3.538356	3.004690	0.661849
H	1.749827	3.504022	-0.410807	C	4.127309	2.161189	1.612734
H	3.824166	0.524238	2.988419	H	4.132209	3.768253	0.170753
H	5.176878	2.278866	1.863329	N	-4.618983	-2.790299	1.275381
C	-5.505638	-3.961772	1.522959	H	-6.129072	-3.756987	2.393047
H	-6.129932	-4.127947	0.642026	H	-4.889579	-4.839030	1.715005

Zero-point correction= 0.360050 (Hartree/Particle)
Thermal correction to Energy= 0.380478
Thermal correction to Enthalpy= 0.381422
Thermal correction to Gibbs Free Energy= 0.307835
Sum of electronic and zero-point Energies= -1017.019718
Sum of electronic and thermal Energies= -1016.999291
Sum of electronic and thermal Enthalpies= -1016.998346
Sum of electronic and thermal Free Energies= -1017.071933

N-Methyl-2,6-Diphenyl-4,4'-Pyrylogen Radical Cation, $2^{+\cdot}$, (B3LYP/6-31+G(d,p))

C	-2.005550	-0.633439	-1.678480	C	-2.292001	0.075714	-2.888115
C	-3.368211	-0.244472	-3.670364	C	-3.990938	-1.966131	-2.186840
C	-2.927878	-1.684197	-1.372769	C	-0.883351	-0.317613	-0.839608
C	-0.598925	-1.039337	0.359887	C	0.482982	-0.732953	1.140702
C	1.079766	1.041501	-0.328426	C	0.024565	0.741026	-1.147451
H	-1.664470	0.888015	-3.230000	H	-3.592503	0.286646	-4.587387
H	-4.695528	-2.757755	-1.962571	H	-2.815810	-2.293306	-0.485878
H	-1.240959	-1.838271	0.701423	H	-0.081600	1.327304	-2.048363
C	-5.411064	-1.541525	-4.159535	H	-6.268168	-0.965235	-3.798083
H	-5.204591	-1.273717	-5.196273	H	-5.641960	-2.606408	-4.110985

C	2.074024	2.098814	-0.532389	C	1.776183	3.221478	-1.329412
C	3.346535	2.001884	0.063503	C	2.732306	4.212315	-1.535607
H	0.788221	3.339814	-1.762836	C	4.299362	2.996191	-0.149245
H	3.590371	1.140837	0.675320	C	3.997505	4.101946	-0.949072
H	2.487381	5.077532	-2.143446	H	5.280123	2.905541	0.306807
C	0.880309	-1.396801	2.385566	C	0.493314	-2.726006	2.645686
C	1.651422	-0.709460	3.342781	C	0.856904	-3.344744	3.838839
H	-0.063204	-3.289865	1.903828	C	2.008796	-1.333938	4.536176
H	1.952031	0.315437	3.156980	C	1.612825	-2.650347	4.789135
H	0.561800	-4.372913	4.022839	H	2.594242	-0.790824	5.271278
N	-4.222838	-1.262030	-3.338833	O	1.303817	0.303297	0.798276
H	1.895538	-3.134938	5.718387	H	4.740926	4.876166	-1.110931

Zero-point correction= 0.358619 (Hartree/Particle)
Thermal correction to Energy= 0.379234
Thermal correction to Enthalpy= 0.380178
Thermal correction to Gibbs Free Energy= 0.305548
Sum of electronic and zero-point Energies= -1017.342157
Sum of electronic and thermal Energies= -1017.321542
Sum of electronic and thermal Enthalpies= -1017.320598
Sum of electronic and thermal Free Energies= -1017.395228

Neutral N-Methyl-2,6-Diphenyl-4,4'-Pyrylogen, 2^0, (B3LYP/6-31+G(d,p))

C	-0.285744	0.477780	0.318780	C	0.410257	-0.634784	0.949610
C	1.473148	-0.455535	1.773064	C	1.354000	1.894403	1.495368
C	0.287867	1.770319	0.666036	C	-1.379824	0.322488	-0.526362
C	-2.065424	1.433362	-1.158545	C	-3.117303	1.263575	-1.994641
C	-3.020101	-1.099430	-1.686920	C	-1.949002	-0.967003	-0.868805
H	0.089356	-1.654982	0.779539	H	1.987490	-1.289233	2.238039
H	1.776575	2.860469	1.748216	H	-0.132744	2.685907	0.269221
H	-1.753604	2.449729	-0.960029	H	-1.508942	-1.876583	-0.483121
C	3.233108	0.947686	2.786969	H	3.255859	1.904801	3.314512
H	3.342544	0.149476	3.525785	C	-3.657437	-2.360568	-2.095378
C	-3.491473	-3.544019	-1.348278	C	-4.454987	-2.413093	-3.255043
C	-4.078106	-4.738010	-1.760931	H	-2.918973	-3.526622	-0.426407
C	-5.043812	-3.610966	-3.662803	H	-4.598274	-1.512020	-3.839884
C	-4.857429	-4.780679	-2.922726	H	-3.938880	-5.636095	-1.165620
H	-5.649240	-3.628420	-4.564807	C	-3.871967	2.325526	-2.677630
C	-3.328710	3.613640	-2.857050	C	-5.166221	2.075456	-3.173559
C	-4.061878	4.618101	-3.484045	H	-2.317523	3.826138	-2.525125
C	-5.895967	3.084137	-3.804606	H	-5.599069	1.089761	-3.049318
C	-5.352278	4.361052	-3.961258	H	-3.619124	5.601636	-3.614290
H	-6.895296	2.869377	-4.172937	N	1.962785	0.801782	2.095006
O	-3.622325	0.002984	-2.272634	H	-5.920258	5.143883	-4.455255
H	-5.318627	-5.711460	-3.239584	H	4.087498	0.906767	2.095781

Zero-point correction= 0.356260 (Hartree/Particle)

Thermal correction to Energy= 0.377158
Thermal correction to Enthalpy= 0.378102
Thermal correction to Gibbs Free Energy= 0.304067
Sum of electronic and zero-point Energies= -1017.530867
Sum of electronic and thermal Energies= -1017.509970
Sum of electronic and thermal Enthalpies= -1017.509026
Sum of electronic and thermal Free Energies= -1017.583061