

Electronic Supplementary Information

On the direct scavenging activity of melatonin towards hydroxyl and a series of peroxy radicals

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Table S1. Gibbs free energies of reaction, in gas phase, at 298.15 k, in kcal/mol.

	R1*	R2	R3	R4	R5
<i>SET</i>	124.62	145.07	123.35	134.55	98.03
<i>HAT/PCET</i>					
C1	-19.55	12.58	13.74	14.40	7.58
C3	-20.92	11.21	12.37	13.02	6.21
C4	-29.49	2.64	3.81	4.46	-2.36
C13	-20.98	11.15	12.31	12.97	6.15
N1	-9.48	22.65	23.81	24.47	17.65
N2	-26.70	5.43	6.59	7.25	0.43
<i>RAF</i>					
C5	-10.00	16.21	17.69	19.70	9.12
C6	-22.75	1.77	6.34	6.83	-0.93
C7	-4.54	22.22	23.75	25.04	16.09
C8	5.43	28.92	29.30	32.06	21.35
C9	-14.77	11.43	12.39	13.69	5.15
C10	-10.77	16.46	17.43	20.91	11.15
C11	-12.52	13.95	15.05	17.62	7.08
C12	-13.95	11.95	13.71	15.35	6.93

*R1=•OH, R2=•OOH, R3=•OO-CH=CH₂, R4=•OO-CH₂-CH=CH₂, R5=•OOCCL₃

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Table S2. Gibbs free energies of activation, in gas-phase, at 298.15 k, in kcal/mol.

	R1*	R2	R3	R4	R5
<i>HAT</i>					
C1	9.99				25.07
C1b	9.90				
C3	7.69				14.99
C4	5.92	20.41	21.23	21.67	16.96
C13	5.11				19.92
N1	11.50				
N2	5.89				12.62
<i>RAF</i>					
C5	4.60				
C6	2.14	18.07			10.24
C7	7.28				
C9	4.14				
C10	6.65				
C11	6.98				
C12	6.21				

*R1=*OH, R2=*OOH, R3=*OO-CH=CH₂, R4=*OO-CH₂-CH=CH₂, R5=*OOCCL₃

Table S3. Electronic charge density $\rho(r)$ and its Laplacian, $\nabla^2\rho(r)$, from Bader topological analyses.

	$\rho(r)$	$\nabla^2\rho(r)$
TS-C1 (R1)	0.01901	-0.01630
TS-C1b (R1)	0.01823	-0.01636
TS-C4 (R1)	0.01763	-0.01591
TS-C13 (R1)	0.02417	-0.02178
TS-C4 (R2)	0.02564	-0.02196
TS-C1 (R5)	0.01428	-0.01344

Optimized geometries in cartesian coordinates, and thermochemistry data from Gaussian03 outputs.

Melatonin

O,3.9591527556,9.
1033147906,5.5573674181\O,-0.2300732499,8.5073536772,7.7031212184\N,0.
3582802817,8.3460313704,1.4816362843\N,-2.2593661019,8.9000145144,6.78
63188795\C,-0.5073368643,8.0719180418,3.5392519604\C,0.8850031336,8.41
13118886,3.6632212055\C,-1.4239057098,7.8303225974,4.6976750369\C,1.39
54957089,8.5746934714,2.3623973294\C,-0.7797174246,8.044969033,2.19650
70068\C,-1.7109816635,9.1347389459,5.4589544968\C,1.7178827097,8.57781
94171,4.7870613203\C,2.7385259277,8.9062378776,2.1429130596\C,3.043330
6044,8.9072766331,4.5620887694\C,3.5475304937,9.0694158432,3.249852671
3\C,-1.4495437087,8.5756179577,7.8242988867\C,-2.1285046695,8.30554680
88,9.1491519917\C,3.4931126935,8.9598828601,6.8896008998\H,-2.36218817
99,7.3775574988,4.3660453693\H,-0.9503192256,7.1341983075,5.3961605157
\H,-1.7053009563,7.8239078463,1.6876044938\H,-2.4105366115,9.757936939
1,4.9008352496\H,-0.785284454,9.6960180282,5.5824977488\H,0.4231577243
,8.3819391487,0.480387727\H,1.3127582753,8.4531734147,5.7830937008\H,3
.1386751127,9.0322279824,1.14396905\H,4.5931480053,9.3270713624,3.1416
042446\H,-3.2556851573,8.8936454526,6.9222830037\H,-3.2074568788,8.460
641158,9.1219062769\H,-1.6874939366,8.9607648451,9.9001036502\H,-1.919
120659,7.2759631442,9.4409016419\H,4.3507026461,9.1581196459,7.5274921
605\H,2.6943148471,9.6735943756,7.1056936258\H,3.1237445315,7.94677512
21,7.0680031065\
Zero-point correction= 0.279986 (Hartree/Particle)
Thermal correction to Energy= 0.296276
Thermal correction to Enthalpy= 0.297220
Thermal correction to Gibbs Free Energy= 0.234898
Sum of electronic and zero-point Energies= -764.638362
Sum of electronic and thermal Energies= -764.622072
Sum of electronic and thermal Enthalpies= -764.621128
Sum of electronic and thermal Free Energies= -764.683450

Melatonin (radical cation)

O,-1.600967
021,2.9034289692,0.0316951103\O,2.3046544238,1.0779776075,-0.136122436
5\N,-2.5437752549,-2.3889538209,-0.0284263109\N,3.1822244065,-0.904315
239,0.4812329045\C,-0.357326184,-1.88896648,-0.2909895758\C,-1.1369819
328,-0.6679413085,-0.1495232828\C,1.1247696812,-1.9113298677,-0.487995
394\C,-2.5066373716,-1.0502836071,0.0104931559\C,-1.2509685685,-2.9074
571935,-0.2105021145\C,1.8781305105,-1.4627973693,0.7850942243\C,-0.77
72010113,0.6557654468,-0.1535834327\C,-3.5486476115,-0.0931644809,0.17
04247479\C,-1.8217713644,1.6131442437,0.0102153033\C,-3.1969227211,1.2
227308181,0.168145516\C,3.3001042398,0.3694791411,0.0395306053\C,4.692
2464352,0.8801572697,-0.2245323783\C,-0.2535072172,3.4197541566,-0.116
7562731\H,1.4569403917,-2.9035005911,-0.7956028862\H,1.3779053951,-1.2
158946263,-1.2921407696\H,-1.1040798449,-3.973665103,-0.2747725851\H,2
.0110601539,-2.3028842506,1.465270478\H,1.3043285105,-0.6967037419,1.3
077668739\H,-3.3770132173,-2.9530347585,0.0548038976\H,0.2617110684,0.
9516987539,-0.2589968041\H,-4.5801844239,-0.3981285946,0.289024151\H,-
3.9279025329,2.0110213202,0.2846702297\H,4.0114399483,-1.4575387293,0.
6207208\H,5.4668053016,0.1396330775,-0.0291112532\H,4.8633013379,1.755
0435222,0.403165452\H,4.7527308193,1.2011231578,-1.2646158682\H,-0.361
9964242,4.4948556889,-0.0359015923\H,0.3811301865,3.0287336466,0.67571
61297\H,0.1371288914,3.1407639425,-1.093279622\
Zero-point correction= 0.280835 (Hartree/Particle)

Thermal correction to Energy= 0.296935
Thermal correction to Enthalpy= 0.297879
Thermal correction to Gibbs Free Energy= 0.235802
Sum of electronic and zero-point Energies= -764.381963
Sum of electronic and thermal Energies= -764.365863
Sum of electronic and thermal Enthalpies= -764.364919
Sum of electronic and thermal Free Energies= -764.426996

Radical OH

\O,0.,0.,0.1111351168\H,0.,0.,-0.8656191168\
Zero-point correction= 0.008468 (Hartree/Particle)
Thermal correction to Energy= 0.010828
Thermal correction to Enthalpy= 0.011772
Thermal correction to Gibbs Free Energy= -0.008463
Sum of electronic and zero-point Energies= -75.708120
Sum of electronic and thermal Energies= -75.705760
Sum of electronic and thermal Enthalpies= -75.704816
Sum of electronic and thermal Free Energies= -75.725051

OH anion

\O,0.,0.,0.1068205216\H,0.,0.,-0.8613045216\
Zero-point correction= 0.008562 (Hartree/Particle)
Thermal correction to Energy= 0.010922
Thermal correction to Enthalpy= 0.011866
Thermal correction to Gibbs Free Energy= -0.007697
Sum of electronic and zero-point Energies= -75.765485
Sum of electronic and thermal Energies= -75.763124
Sum of electronic and thermal Enthalpies= -75.762180
Sum of electronic and thermal Free Energies= -75.781744

H2O

\O,-2.2791160458,0.6495453904,0.\H,-1.3163435161,0.6776711613,0.\H,-2.5739836036,1.5664832979,0.\
Zero-point correction= 0.021510 (Hartree/Particle)
Thermal correction to Energy= 0.024345
Thermal correction to Enthalpy= 0.025289
Thermal correction to Gibbs Free Energy= 0.003869
Sum of electronic and zero-point Energies= -76.383298
Sum of electronic and thermal Energies= -76.380463
Sum of electronic and thermal Enthalpies= -76.379519
Sum of electronic and thermal Free Energies= -76.400939

Radical OOH

\O,-2.0222005857,0.4631381754,-0.0527575\H,-2.3128248784,1.3945538773,-0.0527575\
Zero-point correction= 0.014637 (Hartree/Particle)
Thermal correction to Energy= 0.017488
Thermal correction to Enthalpy= 0.018432
Thermal correction to Gibbs Free Energy= -0.007517
Sum of electronic and zero-point Energies= -150.862873
Sum of electronic and thermal Energies= -150.860022
Sum of electronic and thermal Enthalpies= -150.859077
Sum of electronic and thermal Free Energies= -150.885027

OOH anion

\O,-2.110030719,0.4549689253,-0.0527575\H,-2.3070053459,1.3974140689,-0.0527575\
Zero-point correction= 0.013579 (Hartree/Particle)
Thermal correction to Energy= 0.016480
Thermal correction to Enthalpy= 0.017425
Thermal correction to Gibbs Free Energy= -0.008160
Sum of electronic and zero-point Energies= -150.895328
Sum of electronic and thermal Energies= -150.892426

Sum of electronic and thermal Enthalpies= -150.891482
Sum of electronic and thermal Free Energies= -150.917067

H2O2

\O,0.7070126265,0.

0961518183,-0.1754458999\H,0.998034109,-0.6863509103,0.314579719\O,-0.7070126605,-0.0961516423,-0.1754458626\H,-0.9980340451,0.6863505843,0.3145806236\

Zero-point correction= 0.027247 (Hartree/Particle)
Thermal correction to Energy= 0.030413
Thermal correction to Enthalpy= 0.031357
Thermal correction to Gibbs Free Energy= 0.005016
Sum of electronic and zero-point Energies= -151.487229
Sum of electronic and thermal Energies= -151.484063
Sum of electronic and thermal Enthalpies= -151.483119
Sum of electronic and thermal Free Energies= -151.509459

Radical OO-CH=CH₂

\O,-0.6258972

158,-0.0117361528,-0.0887941785\O,0.6792558497,0.0015352791,-0.0079812568\C,1.1774419506,-1.0847417938,0.6979272823\H,0.4020900604,-1.7438295035,1.0624559647\C,2.4889699032,-1.2031937569,0.8497851051\H,3.1684026539,-0.4715100671,0.4334833301\H,2.891540948,-2.042425255,1.3975990231\

Zero-point correction= 0.048924 (Hartree/Particle)
Thermal correction to Energy= 0.053242
Thermal correction to Enthalpy= 0.054187
Thermal correction to Gibbs Free Energy= 0.021929
Sum of electronic and zero-point Energies= -228.213972
Sum of electronic and thermal Energies= -228.209654
Sum of electronic and thermal Enthalpies= -228.208710
Sum of electronic and thermal Free Energies= -228.240967

OO-CH=CH₂ anion

\O,-0.76908

38228,-0.0709631579,-0.0474079677\O,0.6833406199,0.0022352028,-0.020995132\C,1.1956757155,-1.00472662,0.643836334\H,0.440999956,-1.6903102209,1.0240181675\C,2.5202882988,-1.2046811069,0.8549108052\H,3.265360325,-0.5162864378,0.4752916189\H,2.8452230576,-2.0711689093,1.4148258253\

Zero-point correction= 0.047489 (Hartree/Particle)
Thermal correction to Energy= 0.051914
Thermal correction to Enthalpy= 0.052858
Thermal correction to Gibbs Free Energy= 0.021094
Sum of electronic and zero-point Energies= -228.273890
Sum of electronic and thermal Energies= -228.269465
Sum of electronic and thermal Enthalpies= -228.268520
Sum of electronic and thermal Free Energies= -228.300285

HOO-CH=CH₂

\O,-0.7483342015

,-0.0411854305,0.0646455924\H,-0.7533441017,0.8091459923,0.5310763929\O,0.6365230308,-0.183862353,-0.2364840554\C,1.1575087765,-1.137268518,0.6055559507\H,0.4308026881,-1.864961137,0.9432615641\C,2.454837045,-1.1482773265,0.8860664087\H,3.1178119692,-0.3794351714,0.5121192538\H,2.8667269435,-1.9556613061,1.4738121627\

Zero-point correction= 0.060959 (Hartree/Particle)
Thermal correction to Energy= 0.065747
Thermal correction to Enthalpy= 0.066691
Thermal correction to Gibbs Free Energy= 0.034021
Sum of electronic and zero-point Energies= -228.837063
Sum of electronic and thermal Energies= -228.832276
Sum of electronic and thermal Enthalpies= -228.831332
Sum of electronic and thermal Free Energies= -228.864002

Radical OO-CH₂-CH=CH₂

\O,-0.5090476
471,-0.1530629926,-0.399352908\O,0.7838016386,-0.2823019347,-0.3169604
857\C,1.1584097987,-0.9728619537,0.9109680109\H,0.7697458473,-1.988627
9474,0.8475965155\H,0.6710829681,-0.436069231,1.7251412265\C,2.6482470
541,-0.9407791081,1.0103019857\H,3.1103321916,0.0406693969,1.040058662
7\C,3.3895335845,-2.0435973412,1.078385987\H,2.9397445024,-3.029887075
7,1.0427618628\H,4.4666105718,-1.9951247826,1.1767684925\\
Zero-point correction= 0.078433 (Hartree/Particle)
Thermal correction to Energy= 0.084043
Thermal correction to Enthalpy= 0.084987
Thermal correction to Gibbs Free Energy= 0.048865
Sum of electronic and zero-point Energies= -267.490893
Sum of electronic and thermal Energies= -267.485282
Sum of electronic and thermal Enthalpies= -267.484338
Sum of electronic and thermal Free Energies= -267.520460

OO-CH₂-CH=CH₂ anion

\O,-0.65398
30477,-0.1050366147,-0.2506356789\O,0.8024474617,-0.1408865282,-0.2613
942606\C,1.1590964409,-0.9589867774,0.7975234082\H,0.7747313593,-1.983
6626639,0.6622207478\H,0.712472373,-0.568492495,1.7296855738\C,2.65793
61885,-0.9711176427,0.9254424878\H,3.132998533,0.0019798514,0.81962464
2\C,3.4053743142,-2.0506222553,1.1652074573\H,2.9540617064,-3.03465290
32,1.2516200641\H,4.4833251807,-1.990164941,1.2763749085\\
Zero-point correction= 0.076301 (Hartree/Particle)
Thermal correction to Energy= 0.082019
Thermal correction to Enthalpy= 0.082964
Thermal correction to Gibbs Free Energy= 0.047348
Sum of electronic and zero-point Energies= -267.532797
Sum of electronic and thermal Energies= -267.527079
Sum of electronic and thermal Enthalpies= -267.526135
Sum of electronic and thermal Free Energies= -267.561750

HOO-CH₂-CH=CH₂

\O,-0.6617809808
, -0.1520478862,-0.1006291778\H,-0.8266603773,0.8013570843,-0.060496983
3\O,0.766094495,-0.1787399155,-0.1176224181\C,1.1566002828,-0.96453220
63,1.0084545722\H,0.773286534,-1.9808773707,0.8948318927\H,0.730778678
8,-0.5164453389,1.9114924571\C,2.65380097,-0.9451637747,1.046153862\H,
3.1209166041,0.0319996918,1.1191458494\C,3.3950088773,-2.0497204317,1.
0144064042\H,2.940696751,-3.0310205253,0.9312275081\H,4.4754806552,-2.
0079244568,1.0732859135\\
Zero-point correction= 0.090299 (Hartree/Particle)
Thermal correction to Energy= 0.096484
Thermal correction to Enthalpy= 0.097428
Thermal correction to Gibbs Free Energy= 0.060896
Sum of electronic and zero-point Energies= -268.112878
Sum of electronic and thermal Energies= -268.106694
Sum of electronic and thermal Enthalpies= -268.105750
Sum of electronic and thermal Free Energies= -268.142281

Radical OOCCL₃

\O,0,-0.639241751,0.0992421338,-0.0418
469922\O,0,0.6614114682,0.0859522784,0.0313351142\C,0,1.1510244539,-1.
0810252098,0.7236034852\Cl,0,0.5360029644,-1.0807776817,2.3749017714\C
l,0,0.6461903035,-2.5314145582,-0.1360970817\Cl,0,2.8949481909,-0.8790
024925,0.6848874431\\
Zero-point correction= 0.015106 (Hartree/Particle)
Thermal correction to Energy= 0.021328
Thermal correction to Enthalpy= 0.022273

Thermal correction to Gibbs Free Energy= -0.017012
Sum of electronic and zero-point Energies= -1568.864720
Sum of electronic and thermal Energies= -1568.858498
Sum of electronic and thermal Enthalpies= -1568.857553
Sum of electronic and thermal Free Energies= -1568.896838

OOCCl₃ anion

\O,-0.7246

566296,0.0866433932,-0.031549625\O,0.7226692186,0.079140978,0.03157972
08\C,1.1290161022,-0.9749531617,0.6599684052\Cl,0.5363363274,-1.091436
6429,2.4006028274\Cl,0.6483486713,-2.5638462271,-0.1351400207\Cl,2.938
62194,-0.9225738695,0.7113224323\\

Zero-point correction= 0.014122 (Hartree/Particle)

Thermal correction to Energy= 0.020599
Thermal correction to Enthalpy= 0.021543
Thermal correction to Gibbs Free Energy= -0.017523
Sum of electronic and zero-point Energies= -1568.964737
Sum of electronic and thermal Energies= -1568.958260
Sum of electronic and thermal Enthalpies= -1568.957315
Sum of electronic and thermal Free Energies= -1568.996382

HOCCl₃

\O,-0.6733001

846,0.105490036,-0.0702943938\H,-0.914536259,0.7142035198,0.6489785735
\O,0.7399236335,0.1043344726,0.0264451486\C,1.1454989597,-1.0373578248
,0.697331546\Cl,0.5281542325,-1.0394306038,2.3747472922\Cl,0.615173440
9,-2.5124426453,-0.1291748819\Cl,2.905183787,-0.9132946445,0.693330985
3\\

Zero-point correction= 0.027681 (Hartree/Particle)

Thermal correction to Energy= 0.034221
Thermal correction to Enthalpy= 0.035165
Thermal correction to Gibbs Free Energy= -0.003908
Sum of electronic and zero-point Energies= -1569.498201
Sum of electronic and thermal Energies= -1569.491662
Sum of electronic and thermal Enthalpies= -1569.490717
Sum of electronic and thermal Free Energies= -1569.529790

Product (H transfer from C1)

\O,-1.775597119

9,2.9857504022,0.0492243199\O,2.5968841494,1.1648181986,-0.154280146\N
,2.4893273104,-2.4578705794,-0.0347136807\N,3.2153271576,-0.907168702
9,0.550779801\C,-0.3556383689,-1.8035547929,-0.3126088623\C,-1.1817401
808,-0.6366224731,-0.1546557239\C,1.1283922804,-1.7682323953,-0.502811
2677\C,-2.5064496931,-1.079085026,0.0155409705\C,-1.1946942032,-2.8840
465807,-0.2317294003\C,1.842510301,-1.3220539231,0.78494423\C,-0.87895
66685,0.739119636,-0.1536414629\C,-3.5605433095,-0.1734943191,0.190111
8331\C,-1.925663574,1.6277277501,0.0216541827\C,-3.2549207179,1.173024
7885,0.1914834161\C,3.4872427999,0.3325097268,0.0469824511\C,4.8855375
033,0.6224751232,-0.2266000355\C,-0.4556837464,3.4841906243,-0.0994295
768\H,1.505521604,-2.7449484478,-0.8178928989\H,1.377016162,-1.0490675
349,-1.2887472734\H,-0.9689408876,-3.9365030777,-0.3088428712\H,1.8446
933966,-2.1278636578,1.5197259746\H,1.3144927761,-0.4730439743,1.21819
56893\H,-3.2916217688,-3.0557001403,0.0485429123\H,0.1445097376,1.0675
385129,-0.2816032472\H,-4.5831589126,-0.5070557859,0.3200075606\H,-4.0
280271057,1.9188376695,0.3237228932\H,3.957833075,-1.5831226146,0.6154
951412\H,5.6709638837,-0.1008934787,-0.0565265459\H,5.1291997634,1.599
9250579,-0.6116835834\H,-0.5382118938,4.5664932322,-0.040630833\H,0.19
55966177,3.1156535586,0.6969688164\H,-0.034923547,3.1956769334,-1.0660
721729\\

Zero-point correction= 0.266075 (Hartree/Particle)

Thermal correction to Energy= 0.282078
Thermal correction to Enthalpy= 0.283023

Thermal correction to Gibbs Free Energy= 0.221301
Sum of electronic and zero-point Energies= -763.988292
Sum of electronic and thermal Energies= -763.972288
Sum of electronic and thermal Enthalpies= -763.971344
Sum of electronic and thermal Free Energies= -764.033065

Product (H transfer from C3)

\O,-1.5100853182,3.0537688298,0.0196383956\O,2.5950352883,0
.6856124132,-0.8299120389\N,-2.5969260968,-2.3294934038,0.0342314618\N
,3.0212072088,-0.9038846067,0.7504496955\C,-0.4297742502,-1.8260635338
,-0.2927035535\C,-1.1680047172,-0.6041294912,-0.1274380394\C,1.0538825
153,-1.9155402963,-0.5064343854\C,-2.5169178413,-0.9524787916,0.072624
0127\C,-1.3385410409,-2.8451885024,-0.1879918854\C,1.7983607692,-1.570
9503729,0.746018077\C,-0.7714710144,0.7462424537,-0.1531292074\C,-3.50
17805123,0.0257661144,0.2584780839\C,-1.7509881771,1.7067047028,0.0274
468596\C,-3.1038611894,1.3477730362,0.2348197438\C,3.3634966364,0.1751
091818,-0.0257917659\C,4.7781708806,0.680053619,0.1558746723\C,-0.1714
183149,3.4585430007,-0.2058146222\H,1.3131265717,-2.9374771054,-0.8197
715868\H,1.3557362206,-1.2445408773,-1.310789981\H,-1.1860021908,-3.91
12059807,-0.259506429\H,1.5706018431,-2.1027254246,1.6587859617\H,-3.4
380121953,-2.869549035,0.1286524034\H,0.2681565256,0.9917458764,-0.323
580143\H,-4.5421496139,-0.2344475765,0.413060923\H,-3.8210132345,2.147
0915635,0.3700299103\H,3.6691994496,-1.1431748821,1.4849472239\H,5.268
6655109,0.2889033247,1.0480824535\H,4.7509990296,1.7678249326,0.200260
2223\H,5.3645142272,0.3950581287,-0.7195862258\H,-0.1816107969,4.54546
90961,-0.1918478697\H,0.4880601268,3.0837420532,0.581682742\H,0.189397
5804,3.1019686736,-1.1738195888\

Zero-point correction= 0.265891 (Hartree/Particle)
Thermal correction to Energy= 0.282262
Thermal correction to Enthalpy= 0.283206
Thermal correction to Gibbs Free Energy= 0.220285
Sum of electronic and zero-point Energies= -763.989411
Sum of electronic and thermal Energies= -763.973041
Sum of electronic and thermal Enthalpies= -763.972096
Sum of electronic and thermal Free Energies= -764.035018

Product (H transfer from C4)

\O,0.0453575185,3.1194846351,-0.255430254\O,-3.1712149882,0
.155706433,-0.6266489096\N,3.1389918497,-1.3676476768,0.373449532\N,-2
.0506698834,-1.573515338,0.3105632365\C,1.0241838713,-1.8348251169,-0.
3003189297\C,1.165815751,-0.388165216,-0.1343495081\C,-0.0843812601,-2
.6049644263,-0.7018616675\C,2.4886375484,-0.149678252,0.281890446\C,2.
27668574,-2.3678960818,0.0260161143\C,-1.4524735245,-2.0530795122,-0.9
395707939\C,0.2969546316,0.7028205027,-0.328024183\C,2.9727637296,1.13
80207978,0.5272332621\C,0.7812920561,1.9830118486,-0.0934432622\C,2.10
84094402,2.1967792593,0.336570091\C,-2.8402753787,-0.477029618,0.37307
08809\C,-3.2543351229,-0.0395829654,1.7615173885\C,-1.2805845084,2.976
1015635,-0.74456274\H,0.0559410522,-3.6735869337,-0.8009497693\H,2.587
9673012,-3.399981579,0.0278436018\H,-2.0945987618,-2.8181469437,-1.380
299067\H,-1.4491613207,-1.2060256264,-1.6287350126\H,4.0994563013,-1.4
94014994,0.6391188424\H,-0.7195497983,0.554065182,-0.6591105556\H,3.99
29366457,1.3069870381,0.8502496458\H,2.4270570308,3.2171443064,0.50482
97008\H,-1.7399651914,-2.0035138972,1.1668787504\H,-3.1606451616,-0.83
23274488,2.5042336734\H,-4.2845613487,0.3096216455,1.7222089499\H,-2.6
201035404,0.7984026267,2.0603303791\H,-1.6714823313,3.9857565722,-0.83
71449478\H,-1.286852279,2.4845214913,-1.7201966349\H,-1.899975618,2.39
90805442,-0.0559197395\

Zero-point correction= 0.266423 (Hartree/Particle)
Thermal correction to Energy= 0.282599
Thermal correction to Enthalpy= 0.283544
Thermal correction to Gibbs Free Energy= 0.221404
Sum of electronic and zero-point Energies= -764.003878

Sum of electronic and thermal Energies= -763.987702
Sum of electronic and thermal Enthalpies= -763.986758
Sum of electronic and thermal Free Energies= -764.048898

Product (H transfer from C13)

\O,-1.760541576
3,2.9878166984,-0.0831530131\O,2.6193170724,1.1291131164,-0.1312710814
\N,-2.4872565761,-2.4513321867,0.0290772578\N,3.2222457294,-0.95815254
19,0.4920165164\C,-0.3612812658,-1.8158615327,-0.342128558\C,-1.17739
03945,-0.641025048,-0.1888860689\C,1.1199120207,-1.7924999771,-0.55509
42546\C,-2.4985530797,-1.0730944499,0.0420422945\C,-1.2010235588,-2.88
88510714,-0.201377499\C,1.8487147732,-1.3714844484,0.731823619\C,-0.87
34473226,0.7314337377,-0.2476406092\C,-3.5449058076,-0.1618522599,0.22
77792991\C,-1.9139990198,1.6198159759,-0.0513386552\C,-3.2356441485,1.
1839665758,0.1820795724\C,3.4993518223,0.2933951492,0.0478128354\C,4.9
560006525,0.6094508604,-0.2106020592\C,-0.5105416632,3.5210996825,-0.0
653309117\H,1.4833439061,-2.7678578828,-0.8891804797\H,1.3655415067,-1
.0641101458,-1.3331026418\H,-0.981822253,-3.944214749,-0.2532295017\H,
1.8529180528,-2.1893954486,1.4532112056\H,1.3282808562,-0.5266764868,1
.1823737407\H,-3.2886691508,-3.0430613561,0.1543294575\H,0.1365271386,
1.0631467289,-0.4538723722\H,-4.5625747149,-0.4891102042,0.4029996259\
H,-4.000262239,1.9367607115,0.3225848304\H,3.9693498028,-1.6258774088,
0.5766867236\H,5.6280592528,-0.2113583425,0.0416514366\H,5.2244816071,
1.489648754,0.3732762158\H,5.0728839507,0.8610992117,-1.2650982949\H,0
.2771913378,2.9803268771,0.4417456112\H,-0.5221519714,4.597421801,-0.1
194782106\

Zero-point correction= 0.265578 (Hartree/Particle)
Thermal correction to Energy= 0.281903
Thermal correction to Enthalpy= 0.282847
Thermal correction to Gibbs Free Energy= 0.219368
Sum of electronic and zero-point Energies= -763.988562
Sum of electronic and thermal Energies= -763.972238
Sum of electronic and thermal Enthalpies= -763.971294
Sum of electronic and thermal Free Energies= -764.034773

Product (H transfer from N1)

\O,-1.826470827
3,2.9986713576,0.1015061429\O,2.6831084356,1.0814916877,-0.4185347273\
N,-2.4730476957,-2.4533393653,0.0741428958\N,3.2430189837,-1.065552232
9,0.1220707381\C,-0.388170613,-1.7727454195,-0.4174825198\C,-1.2064384
778,-0.6156350074,-0.1733432977\C,1.0672373527,-1.7316619744,-0.749765
5528\C,-2.5015948942,-1.0746780173,0.128717198\C,-1.2022479026,-2.8644
122242,-0.25362487\C,1.8910752511,-1.3468576539,0.5165753116\C,-0.9231
315158,0.7638829255,-0.1967352472\C,-3.5439806905,-0.1837361301,0.4128
198934\C,-1.9582331388,1.6388833756,0.085845435\C,-3.2573673903,1.1663
907216,0.388078384\C,3.5376650653,0.2805872754,-0.0606035344\C,4.98727
73574,0.638198512,0.1204265202\C,-0.5462044143,3.5217082725,-0.2081137
183\H,1.4233047489,-2.6902013657,-1.1295136492\H,1.2510252133,-0.97487
71967,-1.5149413735\H,-0.9718319009,-3.9137567547,-0.3543945289\H,1.90
13898827,-2.211629662,1.1824647972\H,1.4100314191,-0.499125852,1.00942
81816\H,-3.2589816938,-3.0600809065,0.2242451757\H,0.0777375721,1.1053
31738,-0.4263238157\H,-4.5436226047,-0.5312193692,0.6445873945\H,-4.02
24518297,1.9019134519,0.6000669884\H,5.3593951201,0.2400546428,1.06614
16397\H,5.1028796701,1.7191607747,0.0897418547\H,5.5696640217,0.177704
1115,-0.6801839767\H,-0.6425389326,4.6025417172,-0.1462313783\H,0.2036
344228,3.1746533885,0.5077550604\H,-0.2405969948,3.234230179,-1.217518
4214\

Zero-point correction= 0.265845 (Hartree/Particle)
Thermal correction to Energy= 0.281989
Thermal correction to Enthalpy= 0.282933
Thermal correction to Gibbs Free Energy= 0.219928
Sum of electronic and zero-point Energies= -763.974121

Sum of electronic and thermal Energies= -763.957978
Sum of electronic and thermal Enthalpies= -763.957033
Sum of electronic and thermal Free Energies= -764.020038

Product (H transfer from N2)

\O,-1.787170546
1,2.9980519464,0.0619804518\O,2.5729394631,1.1099325136,-0.2132327724\
N,-2.5175423914,-2.4963623538,-0.034122882\N,3.2105035082,-0.926053961
8,0.5266319553\C,-0.3534029637,-1.777720778,-0.3272431183\C,-1.1673540
163,-0.6031361011,-0.1615433221\C,1.1203114758,-1.7865708549,-0.513824
0537\C,-2.4796852154,-1.0844260516,0.0144220226\C,-1.2754730374,-2.875
4190582,-0.232383265\C,1.8427162939,-1.3431314104,0.7783115643\C,-0.86
58741259,0.758370368,-0.1588734509\C,-3.5268898262,-0.1999403098,0.198
5519142\C,-1.9359801677,1.644993788,0.0314419573\C,-3.2417264298,1.170
1075796,0.2063588822\C,3.4709499276,0.3076312242,0.0245449437\C,4.9234
441303,0.6430447456,-0.2246169914\C,-0.4736569045,3.513054456,-0.10468
54039\H,1.4746264712,-2.772478879,-0.8224238998\H,1.3832930889,-1.0674
662459,-1.2955957042\H,-1.0143132178,-3.9229886493,-0.3152120916\H,1.8
546390211,-2.1532217797,1.5069499694\H,1.3147483154,-0.4973674284,1.21
73500702\H,0.1527943552,1.0998288915,-0.2943842934\H,-4.5399115551,-0.
5574363077,0.3328977334\H,-4.027677351,1.9004804842,0.3486763467\H,3.9
685394045,-1.5698761689,0.6751937276\H,5.6078138898,-0.1490251047,0.07
99357749\H,5.1624116037,1.556978823,0.3188639879\H,5.0541744933,0.8441
594215,-1.2882512141\H,-0.5706892255,4.5934796559,-0.0417172681\H,0.19
26484554,3.1531304217,0.682776373\H,-0.0646389236,3.2339701242,-1.0786
499437\

Zero-point correction= 0.266102 (Hartree/Particle)
Thermal correction to Energy= 0.282179
Thermal correction to Enthalpy= 0.283123
Thermal correction to Gibbs Free Energy= 0.220358
Sum of electronic and zero-point Energies= -764.001840
Sum of electronic and thermal Energies= -763.985762
Sum of electronic and thermal Enthalpies= -763.984818
Sum of electronic and thermal Free Energies= -764.047584

Product (*OH addition to C5)

\O,-1.629217314
4,2.9648058093,-0.0210905266\O,2.0303459631,1.2950508665,-1.8016169144\
\N,-2.6056649209,-2.4673292779,-0.0620012279\N,2.9578071792,-0.7668229
768,-1.710879484\C,-0.310350499,-1.9252857751,-0.1203100192\C,-1.18116
09675,-0.6779319339,-0.0632252825\C,0.8127450132,-1.8885891161,-1.1613
773639\C,-2.5189065898,-1.0653179415,-0.0018863806\C,-1.3526956568,-2.
9753217592,-0.3800772965\C,2.0920342292,-1.2219417231,-0.6324760056\C,
-0.8264615308,0.6673604402,-0.0706600263\C,-3.5397569318,-0.12399327,0
.0878058557\C,-1.8473684101,1.6189730608,0.0009098561\C,-3.187947533,1
.2205796179,0.0923786696\C,2.8382061618,0.4768412663,-2.233639316\C,3.
7619611243,0.815130805,-3.3830736465\C,-0.283593959,3.399676827,-0.167
6343041\H,1.0408498638,-2.9105202694,-1.4789560013\H,0.4521885331,-1.3
421236572,-2.0349092995\H,-1.161336966,-4.0364624577,-0.3233948737\H,2
.649767217,-1.9134321382,-0.0042248761\H,1.8552939335,-0.3534579925,-0
.0243625196\H,-3.45053734,-2.9217028777,-0.3685422855\H,0.2065485838,0
.9637712624,-0.1830648938\H,-4.580780754,-0.4194460897,0.1399825046\H,
-3.9452400259,1.9919852765,0.1488653104\H,3.6081225595,-1.4104745691,-
2.128864458\H,4.4618351118,0.015027834,-3.6260157239\H,4.3177656939,1.
7159014917,-3.1233023338\H,3.1533004591,1.0402073119,-4.2593785078\H,-
0.3279527241,4.4851756425,-0.1997535201\H,0.3209712237,3.0825250507,0.
6864741114\H,0.1602897391,3.0132089154,-1.0865943762\O,0.3606162651,-2
.1602570425,1.1487975242\H,-0.314049741,-2.1480977004,1.8415530114\

Zero-point correction= 0.294087 (Hartree/Particle)
Thermal correction to Energy= 0.311886
Thermal correction to Enthalpy= 0.312830
Thermal correction to Gibbs Free Energy= 0.247451

Sum of electronic and zero-point Energies= -840.378367
Sum of electronic and thermal Energies= -840.360568
Sum of electronic and thermal Enthalpies= -840.359624
Sum of electronic and thermal Free Energies= -840.425003

Product (*OH addition to C6)

O, -1.774040012

4,3.0165658819,0.093145664\O,2.6046271972,1.1799953521,-0.1162013673\N
,-2.5780912135,-2.4429457302,-0.1996314713\N,3.2035356644,-0.910638154
4,0.4999415616\C,-0.3779460035,-1.7255712336,-0.3811170527\C,-1.199286
5527,-0.6061197905,-0.2215399754\C,1.0982626485,-1.7055197572,-0.56922
28888\C,-2.5376735581,-1.0573451889,-0.0533691897\C,-1.2179612546,-2.9
698472289,-0.2485117159\C,1.8286616719,-1.3202554291,0.7348138566\C,-0
.8919705647,0.7755186904,-0.1978845778\C,-3.5665872756,-0.1541966473,0
.1642958348\C,-1.9307999985,1.663067803,0.0245175298\C,-3.2540791098,1
.2050226542,0.2084716155\C,3.4834357457,0.3404890061,0.0561712479\C,4.
9393625079,0.6526888802,-0.2084113285\C,-0.4547832749,3.5167798628,-0.
0628254868\H,1.4527664024,-2.67449229,-0.9294848479\H,1.3590437976,-0.
9522056451,-1.3192356228\H,1.8324613294,-2.1541484314,1.4374229879\H,1
.3141968425,-0.4814888416,1.202506712\H,-3.272068242,-2.9712935898,0.3
051088492\H,0.1331839139,1.0987952283,-0.3241422981\H,-4.5906334579,-0
.4841155723,0.2891799879\H,-4.0239795436,1.945259227,0.3806712183\H,3.
9450627507,-1.5870275977,0.563689321\H,5.6085872586,-0.1761769358,0.02
33093919\H,5.2182223879,1.520409095,0.3893079317\H,5.0489498133,0.9230
493483,-1.2590002526\H,-0.5329836577,4.59622526,0.0364995352\H,0.21024
03654,3.1178125121,0.7068983094\H,-0.0551010507,3.2626785594,-1.047642
3511\H,-0.9755490483,-3.5438580863,0.6539049378\O,-1.0402900673,-3.909
7876758,-1.2948107962\H,-1.3340208216,-3.4782290549,-2.1105175596\

Zero-point correction= 0.294632 (Hartree/Particle)

Thermal correction to Energy= 0.312428
Thermal correction to Enthalpy= 0.313372
Thermal correction to Gibbs Free Energy= 0.247073
Sum of electronic and zero-point Energies= -840.397748
Sum of electronic and thermal Energies= -840.379953
Sum of electronic and thermal Enthalpies= -840.379009
Sum of electronic and thermal Free Energies= -840.445308

Product (*OH addition to C7)

O, -1.3234630936,3.1696534663,-0.0329190161\O,2.8370201743,

1.031599428,-0.0027919623\N,-2.5565414745,-2.1452575461,-0.5228922108\
N,3.3239319968,-1.1394107117,0.4005788426\C,-0.3121346253,-1.663349145
3,-0.4764909552\C,-1.0126132095,-0.4740049545,-0.1124957771\C,1.166829
6174,-1.7254447254,-0.6968691874\C,-2.4425228136,-0.859214834,0.145776
7179\C,-1.2577536684,-2.6284110645,-0.682333061\C,1.9317584003,-1.5029
375699,0.6178383627\C,-0.5960864906,0.8514452428,-0.0653810215\C,-3.39
75931734,0.2198344483,-0.2458107366\C,-1.5786496744,1.8394969583,-0.07
63402469\C,-2.9697669095,1.5046236287,-0.2465638869\C,3.6686604521,0.1
316487962,0.0801021518\C,5.1383177453,0.389912989,-0.1678781972\C,0.03
99908197,3.5635184494,0.0730866995\H,1.455652561,-2.6801952556,-1.1434
706405\H,1.4609477795,-0.9327853251,-1.3920259906\H,-1.1041240899,-3.6
434604801,-1.0200528332\H,1.9008830385,-2.3995643854,1.2369559239\H,1.
4657580075,-0.6931606884,1.1781502687\H,-3.2298233777,-2.7683021363,-0
.0969492903\H,0.4586985505,1.0912701877,-0.1217215366\H,-4.437022914,-0
.0385364858,-0.4043727172\H,-3.653083396,2.3282419183,-0.4137401033\H,
4.0337683391,-1.8517424226,0.4090978759\H,5.2590353347,0.7380325798,-1
.194106845\H,5.764841109,-0.4879865932,-0.0084959653\H,5.4626646744,1.
1911290461,0.495945816\H,0.0296176511,4.6475431286,0.1433725351\H,0.49
8306284,3.1318270992,0.9650753468\H,0.6040943415,3.2506451364,-0.80748
09498\O,-2.6422290876,-1.1620347475,1.559764454\H,-2.5641142833,-0.32
60868218,2.0421218856\

Zero-point correction= 0.293970 (Hartree/Particle)

Thermal correction to Energy= 0.311696

Thermal correction to Enthalpy= 0.312641
Thermal correction to Gibbs Free Energy= 0.247227
Sum of electronic and zero-point Energies= -840.369217
Sum of electronic and thermal Energies= -840.351490
Sum of electronic and thermal Enthalpies= -840.350546
Sum of electronic and thermal Free Energies= -840.415960

Product (*OH addition to C8)

\O,-1.6692482156,3.0482455098,-0.1034687228\O,2.720132213,1
.1725043257,-0.1131736002\N,-2.5366938041,-2.3202307253,-0.4329268819
N,3.3088438543,-0.967194049,0.3188623656\C,-0.3355075377,-1.6984443527
,-0.4470115652\C,-1.1179449281,-0.622916538,0.2887461791\C,1.137933584
4,-1.6168864633,-0.6795730218\C,-2.53439837,-0.9864882161,-0.062068678
6\C,-1.2058286177,-2.6621893333,-0.7849256788\C,1.9415463901,-1.375005
2996,0.6081231204\C,-0.7982751019,0.8072236494,0.0286945184\C,-3.55330
4509,-0.058364437,-0.0525825738\C,-1.8198910961,1.6974805782,-0.000173
6419\C,-3.2034675037,1.2877779459,0.0365540551\C,3.5903894414,0.310422
2952,-0.0378305971\C,5.0406526023,0.6228849058,-0.3356346437\C,-0.3345
569941,3.5318756769,-0.1281006701\H,1.4967097434,-2.519383046,-1.18267
47849\H,1.3338511475,-0.7695321112,-1.3446920009\H,-1.0161471064,-3.61
61696484,-1.255676725\H,1.9723189681,-2.2766488163,1.2209109404\H,1.47
4148252,-0.5906115708,1.1994765096\H,-3.3089215078,-2.6976483759,-0.95
8683515\H,0.2437817624,1.0963326691,-0.0009370516\H,-4.58878596,-0.350
2712878,-0.1825663509\H,-3.9535535573,2.0655047642,0.0439363196\H,4.04
75810093,-1.6493148587,0.3234751905\H,5.1138000232,0.9776337412,-1.363
9471329\H,5.7043954977,-0.2314340312,-0.1997316975\H,5.3574984078,1.43
40145386,0.3199297442\H,-0.4102739665,4.6143810674,-0.1866958675\H,0.1
99045395,3.2395719582,0.7791507056\H,0.202407614,3.1463737777,-0.99792
92417\O,-0.9208726198,-0.8218190333,1.7338125026\H,-1.1483507101,-1.74
44448193,1.9266041426\

Zero-point correction= 0.293515 (Hartree/Particle)
Thermal correction to Energy= 0.311373
Thermal correction to Enthalpy= 0.312317
Thermal correction to Gibbs Free Energy= 0.246793
Sum of electronic and zero-point Energies= -840.352896
Sum of electronic and thermal Energies= -840.335039
Sum of electronic and thermal Enthalpies= -840.334094
Sum of electronic and thermal Free Energies= -840.399619

Product (*OH addition to C9)

\O,-1.738756540
1,2.9999939776,-0.0467982931\O,2.5424997584,1.1717762918,0.3469122215\
N,-2.4588715306,-2.4444008167,0.1178176593\N,3.2151534136,-0.985771240
3,0.4905845908\C,-0.3597931928,-1.8300698257,-0.3560621526\C,-1.169403
2089,-0.6686795813,-0.236671129\C,1.1188061647,-1.7946743802,-0.596794
0191\C,-2.4651028259,-1.0706943017,0.0591517876\C,-1.1879629221,-2.910
3192588,-0.1280392861\C,1.8693662754,-1.4881585433,0.7123230338\C,-0.8
08088452,0.7567620085,-0.4820777159\C,-3.526592526,-0.1556503469,0.294
7632306\C,-1.9306624508,1.6602573643,-0.0398718096\C,-3.2062136034,1.2
076113699,0.2499149518\C,3.4384534564,0.3369032734,0.2789775915\C,4.86
31063532,0.7329464196,-0.040919817\C,-0.3985842388,3.498021461,-0.1062
556644\H,1.4770701282,-2.7356504939,-1.022658055\H,1.3393269211,-0.997
8552797,-1.3116969978\H,-0.9739541787,-3.9671871541,-0.1287847567\H,1.
925947527,-2.378574119,1.3402692911\H,1.331571601,-0.7208756994,1.2673
105952\H,-3.2555761971,-3.0190624615,0.3296329337\H,0.1331524198,1.016
4410794,0.00524711435\H,-4.52883874,-0.486131521,0.5284577589\H,-3.9621
469937,1.9530770618,0.4632490154\H,3.9715467413,-1.6341572024,0.351641
8964\H,5.5661817536,-0.0987156329,0.0143750639\H,5.168169782,1.5128814
139,0.6563085225\H,4.8841300834,1.1566217969,-1.0456684989\H,-0.497996
1185,4.5799963682,-0.1264199512\H,0.1635473708,3.1963238544,0.77951316
95\H,0.1063363319,3.1463837543,-1.0044996955\O,-0.5231377377,0.9957345
786,-1.8868651244\H,-1.2878038245,0.6718499752,-2.3835380504\

Zero-point correction= 0.294535 (Hartree/Particle)
Thermal correction to Energy= 0.312489
Thermal correction to Enthalpy= 0.313433
Thermal correction to Gibbs Free Energy= 0.247262
Sum of electronic and zero-point Energies= -840.385449
Sum of electronic and thermal Energies= -840.367495
Sum of electronic and thermal Enthalpies= -840.366550
Sum of electronic and thermal Free Energies= -840.432721

Product (*OH addition to C10)

\O,-2.049611432
5,2.7650206495,-0.3546352532\O,2.7272857292,1.0487938103,0.0861497924\
N,-2.4658876318,-2.4239214415,-0.2801659294\N,3.2757998686,-1.10198053
56,0.5052996229\C,-0.3277453153,-1.7527388599,-0.4481408436\C,-1.14935
06853,-0.6189582794,-0.07664485\C,1.1536672562,-1.6991726248,-0.647302
615\C,-2.4770137358,-1.0899014785,0.0147442642\C,-1.1698304664,-2.8234
971386,-0.5613508848\C,1.8892574323,-1.5004577036,0.6874540626\C,-0.84
50722335,0.7139771093,0.1688433401\C,-3.5693111474,-0.2349329199,0.359
8316184\C,-1.9344195677,1.6817267041,0.5379268446\C,-3.3117786713,1.06
90564736,0.5927602057\C,3.5875295334,0.1811182661,0.1912161141\C,5.053
7740047,0.4870028814,-0.0202002996\C,-0.8574613425,3.5152604576,-0.570
5168176\H,1.5121185365,-2.6086212118,-1.1367158737\H,1.4014999816,-0.8
532816799,-1.2941833431\H,-0.9568706507,-3.8455113785,-0.8324226403\H,
1.8670886216,-2.4178528382,1.2765292887\H,1.3945306291,-0.7172172151,1
.2617051356\H,-3.2745888704,-3.0195634301,-0.3119633326\H,0.1724876913
,1.0838867526,0.1238915238\H,-4.5782620028,-0.625138132,0.4285896708\H
, -4.0959269864,1.7685269708,0.8518159457\H,4.0052759187,-1.7932767604,
0.5347024755\H,5.7053801771,-0.3668887038,0.1674790951\H,5.3316846784,
1.3072882832,0.6413503586\H,5.1909470979,0.8267938246,-1.0472549355\H,
-1.1701968435,4.428963425,-1.0713609668\H,-0.3768779205,3.76106734,0.3
766505408\H,-0.1615385739,2.9715785942,-1.2135250208\O,-1.640158271,2.
2687589809,1.8204737172\H,-1.2779684376,1.5738351187,2.3855680192\
Zero-point correction= 0.293085 (Hartree/Particle)
Thermal correction to Energy= 0.311208
Thermal correction to Enthalpy= 0.312152
Thermal correction to Gibbs Free Energy= 0.244540
Sum of electronic and zero-point Energies= -840.377844
Sum of electronic and thermal Energies= -840.359721
Sum of electronic and thermal Enthalpies= -840.358777
Sum of electronic and thermal Free Energies= -840.426390

Product (*OH addition to C11)

\O,-1.769545056
8,2.9708601211,-0.0200326985\O,2.5994560448,1.1519361833,-0.1832594701
\N,-2.5051107522,-2.4834323066,-0.0968658595\N,3.1946535237,-0.8987511
298,0.5588572717\C,-0.3710509571,-1.8016187703,-0.3269837298\C,-1.1901
054455,-0.6577421041,-0.1612382065\C,1.1161898081,-1.7672729144,-0.503
0411382\C,-2.5356505675,-1.098216931,-0.0141217305\C,-1.2086800617,-2.
9015314963,-0.2816204077\C,1.8174577803,-1.3087962023,0.7858918815\C,-
0.8805016114,0.7429687497,-0.1688638327\C,-3.5918781772,-0.2364759428,
0.1506458653\C,-1.8947328488,1.6259990961,0.0093327007\C,-3.3202176577
,1.2270810782,0.3230319318\C,3.4782368715,0.3304958488,0.060334357\C,4
.9397224456,0.6411949782,-0.175634416\C,-0.4612008225,3.4877687809,-0.
2196878691\H,1.4957053621,-2.7466281952,-0.8061146599\H,1.3722595749,-
1.0556254479,-1.2929032145\H,-0.9718974827,-3.9494936076,-0.3770551006
\H,1.8119402566,-2.1061054078,1.5299687561\H,1.2864107225,-0.454179383
6,1.2040800781\H,-3.3070757802,-3.0841798066,-0.0329896732\H,0.1407898
986,1.0613486952,-0.3357913408\H,-4.6153843896,-0.5709561328,0.2573931
086\H,-3.984606509,1.8302590689,-0.2998208987\H,3.9425292814,-1.556740
5794,0.6965860316\H,5.6082265839,-0.1625484279,0.1340455455\H,5.189610
0066,1.5502814745,0.3711144462\H,5.0833133439,0.8411893011,-1.23781959
71\H,-0.5611622056,4.5692848979,-0.1949574818\H,0.2110362004,3.1517031

873,0.5729336316\H,-0.0637939569,3.1681559747,-1.1860233638\O,-3.65986
06498,1.6489770198,1.6621789796\H,-3.1484444124,1.0958127607,2.2688444
937\

Zero-point correction= 0.294236 (Hartree/Particle)
Thermal correction to Energy= 0.312336
Thermal correction to Enthalpy= 0.313280
Thermal correction to Gibbs Free Energy= 0.246252
Sum of electronic and zero-point Energies= -840.380780
Sum of electronic and thermal Energies= -840.362679
Sum of electronic and thermal Enthalpies= -840.361735
Sum of electronic and thermal Free Energies= -840.428764

Product (*OH addition to C12)

\O,-1.701774157
7,2.9828440311,0.1036102936\O,2.5520486817,1.1586081335,-0.1670562486\
N,-2.4752146688,-2.4630076564,-0.0256696044\N,3.2167893247,-0.89488403
95,0.5044878948\C,-0.3484343229,-1.8345043673,-0.3230478531\C,-1.17255
82657,-0.6670658557,-0.1730348814\C,1.1351310784,-1.799166553,-0.52311
73484\C,-2.475182214,-1.1015747521,0.0098227777\C,-1.1872704553,-2.917
5205209,-0.2182554092\C,1.8562683747,-1.3448705599,0.7570862539\C,-0.8
500249519,0.7211576055,-0.1701803854\C,-3.655595159,-0.2150760083,0.20
15254509\C,-1.9109232688,1.6304663222,0.0496492515\C,-3.2122678974,1.2
17315746,0.2272465917\C,3.4569919891,0.352630764,0.0318149321\C,4.9027
736127,0.7069394715,-0.235814835\C,-0.3753657869,3.4517914106,-0.08952
32374\H,1.5108667993,-2.7763510117,-0.8371950527\H,1.3773992571,-1.083
3431374,-1.3136460822\H,-0.9726222618,-3.9729298371,-0.2708232492\H,1.
8890564589,-2.1543026172,1.4869989185\H,1.3146907007,-0.5111403579,1.2
035106005\H,-3.2834507114,-3.0365872969,0.1474692802\H,0.1723045902,1.
0431414793,-0.3061043281\H,-4.3881717535,-0.3681877033,-0.5993971631\H
,-3.9776915822,1.9665036707,0.3821768071\H,3.9849508552,-1.5350476335,
0.611633129\H,5.6000257912,-0.0864336565,0.0346159166\H,5.1446113925,1.
.6086828129,0.3264794796\H,5.0109522856,0.9366806903,-1.2961940659\H,-
0.4331936042,4.5340766628,-0.0058216479\H,0.301982455,3.0574822636,0.6
713829665\H,-0.0000726879,3.1790482824,-1.078832325\O,-4.4032054082,-0
.576347945,1.3824361369\H,-3.8636610295,-0.3226339465,2.1448460162\

Zero-point correction= 0.293990 (Hartree/Particle)
Thermal correction to Energy= 0.312117
Thermal correction to Enthalpy= 0.313062
Thermal correction to Gibbs Free Energy= 0.245718
Sum of electronic and zero-point Energies= -840.383425
Sum of electronic and thermal Energies= -840.365298
Sum of electronic and thermal Enthalpies= -840.364353
Sum of electronic and thermal Free Energies= -840.431697

Product (*OOH addition to C5)

\O,-1.325764630
9,3.2315362408,0.2248185175\O,2.5583409927,1.2032047835,-0.2161933417\
N,-2.6883383909,-2.0538572477,-0.5813188154\N,3.2036759014,-0.93900207
91,0.1162295367\C,-0.526542124,-1.7621756113,0.3175861527\C,-1.2350260
489,-0.4342244064,0.1271422952\C,0.9142319583,-1.829719382,-0.21215465
12\C,-2.5050509223,-0.6708398143,-0.3918854058\C,-1.4818665095,-2.6915
770098,-0.3592177185\C,1.9659034474,-1.31179521,0.7842652133\C,-0.7877
386758,0.8616013738,0.3564663543\C,-3.3820577984,0.3727627145,-0.66390
73048\C,-1.655200678,1.9181727311,0.0672823393\C,-2.9424372236,1.66954
81175,-0.4270951267\C,3.3952880842,0.3167941657,-0.357978218\C,4.70468
05795,0.5737804743,-1.0706504075\C,-0.0069558523,3.5203816254,0.670464
0881\H,1.1490150741,-2.8628139943,-0.4843292279\H,0.9569990144,-1.2271
100252,-1.1210938223\H,-1.3857218012,-3.7632940713,-0.4307199553\H,2.1
896454644,-2.0674503961,1.5348155814\H,1.6066960966,-0.4306049826,1.30
83945269\H,-3.351450239,-2.400688995,-1.2557783679\H,0.218034166,1.045
6971184,0.7038217375\H,-4.3747808204,0.1918052789,-1.0581805073\H,-3.5
806222519,2.5189968777,-0.6333116919\H,3.9064981379,-1.6382131193,-0.0

532509967\H,5.3672745036,-0.2920030676,-1.0840780257\H,5.2066395569,1.
4062005201,-0.577623175\H,4.4854659713,0.8763340425,-2.0949696711\H,0.
0648571872,4.6046761984,0.6906723388\H,0.1562809991,3.1235889012,1.676
1650906\H,0.7401072769,3.1060763631,-0.0090326321\O,-0.3591867056,-2.1
067719852,1.7340270826\O,-1.6120445407,-2.0084783011,2.3892502045\H,-2
.0290558585,-2.8563002585,2.1646893532\

Zero-point correction= 0.297001 (Hartree/Particle)
Thermal correction to Energy= 0.316272
Thermal correction to Enthalpy= 0.317217
Thermal correction to Gibbs Free Energy= 0.247995
Sum of electronic and zero-point Energies= -915.492182
Sum of electronic and thermal Energies= -915.472910
Sum of electronic and thermal Enthalpies= -915.471966
Sum of electronic and thermal Free Energies= -915.541188

Product (*OOH addition to C6)

\O,1.2553808167
,3.3973505398,0.1214539017\O,-2.7985573856,1.0538248839,0.1631992945\N
,2.767192993,-1.921912303,-0.096330279\N,-3.207070634,-1.0270169324,-0
.6204247027\C,0.4771992595,-1.5041094162,0.0425671582\C,1.153978392,-0
.2785689012,0.0310225386\C,-0.9794378923,-1.697724536,0.2677342456\C,2
.5417289949,-0.5336627924,-0.1093903469\C,1.4801822887,-2.6053292095,-
0.1495831967\C,-1.8120807033,-1.2605131973,-0.9555038237\C,0.668001702
8,1.0446211739,0.1355912211\C,3.451250585,0.5070887107,-0.182991544\C,
1.5886799714,2.0773265626,0.0551422797\C,2.9650705289,1.8139919572,-0.
1097035302\C,-3.5907729864,0.1386503949,-0.0418008066\C,-5.0508876629,
0.256882493,0.332771459\C,-0.122435796,3.7029989957,0.2826506345\H,-1.
1917537193,-2.7380934072,0.524639079\H,-1.2903162099,-1.0780231486,1.1
147737261\H,-1.7680711924,-2.0121104884,-1.744422264\H,-1.4142310826,-
0.327071825,-1.3522431875\H,3.4956664562,-2.2814658656,-0.6947675895\H
, -0.3938257825,1.2176114771,0.2541839899\H,4.5141130574,0.3241332947,-
0.2840433486\H,3.6373997896,2.6594529732,-0.1677240258\H,-3.87254895,-
1.7768253426,-0.7007184765\H,-5.6418649987,-0.6139260246,0.0480481588\
H,-5.4586955739,1.144803733,-0.1501030551\H,-5.1191878488,0.4028236708
,1.4112518352\H,-0.1838041773,4.7876432667,0.3086912796\H,-0.710245141
1,3.3150764408,-0.5525351826\H,-0.5081795069,3.2857529935,1.2157543733
\H,1.3468558329,-3.1751690162,-1.0780474024\O,1.4033939972,-3.64590405
94,0.822901167\O,1.5030125645,-3.0470020167,2.1077684541\H,2.420245883
3,-2.7176352495,2.0935854755\

Zero-point correction= 0.298391 (Hartree/Particle)
Thermal correction to Energy= 0.317247
Thermal correction to Enthalpy= 0.318191
Thermal correction to Gibbs Free Energy= 0.247017
Sum of electronic and zero-point Energies= -915.513500
Sum of electronic and thermal Energies= -915.494644
Sum of electronic and thermal Enthalpies= -915.493700
Sum of electronic and thermal Free Energies= -915.564874

Product (*OOH addition to C7)

\O,-1.3369192162,3.151711349,-0.049493044
6\O,2.8146093294,1.0398586695,-0.0848377012\N,-2.5491820491,-2.1588018
292,-0.5170120726\N,3.3141129126,-1.1015241105,0.4410249482\C,-0.30585
54221,-1.682950936,-0.455080919\C,-1.012051318,-0.4870757216,-0.105215
1726\C,1.1750884661,-1.7403159091,-0.6593310763\C,-2.4308803458,-0.878
596342,0.1467859248\C,-1.2464789606,-2.6486764152,-0.6611008773\C,1.92
19946536,-1.4669482747,0.6564701649\C,-0.6029035437,0.8368192651,-0.09
93125452\C,-3.4070417018,0.1944898182,-0.1673247688\C,-1.5885299661,1.
8220527155,-0.0747810373\C,-2.9833574724,1.4824849924,-0.179422137\C,3
.6535984558,0.1554440885,0.0658833212\C,5.126475085,0.4192381618,-0.15
57474147\C,0.0283141047,3.5509277926,0.0258744183\H,1.4762619191,-2.70
67788699,-1.070899735\H,1.4693456752,-0.9683829033,-1.3772548381\H,-1.
0940931556,-3.6670276886,-0.9883215271\H,1.8913207165,-2.3430184766,1.

3040992104\H,1.4416815198,-0.6446797543,1.1858769154\H,-3.2411525209,-
2.7831427223,-0.1241185571\H,0.4487856897,1.0792989826,-0.1903561541\H
,-4.4504032611,-0.0668349156,-0.2948559042\H,-3.6766720793,2.303300135
2,-0.3199239312\H,4.0325522594,-1.8009622979,0.5174646201\H,5.26802098
51,0.7402686292,-1.1879973985\H,5.7561943212,-0.4484470421,0.042281487
6\H,5.4290960731,1.240994861,0.4932530583\H,0.0147123581,4.6347729501,
0.0971763437\H,0.5067845937,3.1193251285,0.9067576406\H,0.5724338197,3
.2411752411,-0.8681109901\O,-2.6129559251,-1.2768549619,1.581224053\O,
-2.2649632618,-0.1965870266,2.4271331662\H,-3.0631486187,0.3564857172,
2.4002197995\

Zero-point correction= 0.297487 (Hartree/Particle)
Thermal correction to Energy= 0.316394
Thermal correction to Enthalpy= 0.317339
Thermal correction to Gibbs Free Energy= 0.249386
Sum of electronic and zero-point Energies= -915.483162
Sum of electronic and thermal Energies= -915.464254
Sum of electronic and thermal Enthalpies= -915.463310
Sum of electronic and thermal Free Energies= -915.531262

Product (*OOH addition to C8)

\O,-1.7302290607,3.0388527945,-0.09064108
33\O,2.7650838777,1.1422347994,-0.1682024288\N,-2.4930460776,-2.322944
4269,-0.4512590372\N,3.3363245768,-0.9808962624,0.3589858983\C,-0.2970
679421,-1.6973494371,-0.4546126201\C,-1.0846748577,-0.6107043547,0.235
8435498\C,1.1800144676,-1.6276278427,-0.665888155\C,-2.5020962557,-1.0
124974979,-0.0368459387\C,-1.1624209392,-2.6636964981,-0.7912995275\C,
1.9604793595,-1.3715088837,0.6329910817\C,-0.8008336763,0.8180487707,-
0.0530779808\C,-3.5400533942,-0.1032028206,0.0683901553\C,-1.841882453
1,1.6872393536,0.0130411428\C,-3.2096993111,1.2451633758,0.1568382622\
C,3.6309598796,0.281586418,-0.0351928371\C,5.0900600009,0.5820208023,-
0.3014381188\C,-0.4124792487,3.5552437024,-0.216615761\H,1.5380520129,
-2.5435172275,-1.1442680958\H,1.3979646745,-0.7957131588,-1.3433685904
\H,-0.9670971466,-3.6201951291,-1.2535603906\H,1.9659383673,-2.2598026
802,1.2642549521\H,1.4922834893,-0.5692431108,1.1986824548\H,-3.273473
7958,-2.7177908784,-0.950812614\H,0.2318624378,1.1203427288,-0.1642845
91\H,-4.5764265875,-0.4128634159,0.0021044946\H,-3.9716021385,2.007510
1407,0.235245062\H,4.0740961781,-1.6611683564,0.4209337971\H,5.1938359
535,0.9021817391,-1.3384135671\H,5.7473965474,-0.2684092342,-0.1181060
829\H,5.3900048812,1.4139099605,0.3358553226\H,-0.5178751334,4.6361622
05,-0.2497773751\H,0.200361781,3.260865478,0.6381181853\H,0.0566811534
,3.1968891514,-1.135701003\O,-0.8414732015,-0.6656353779,1.7159614542\
O,-1.0464608509,-1.9924188382,2.1992380949\H,-1.9549517377,-1.93618309
87,2.5331668705\

Zero-point correction= 0.296897 (Hartree/Particle)
Thermal correction to Energy= 0.316149
Thermal correction to Enthalpy= 0.317093
Thermal correction to Gibbs Free Energy= 0.248099
Sum of electronic and zero-point Energies= -915.471905
Sum of electronic and thermal Energies= -915.452654
Sum of electronic and thermal Enthalpies= -915.451709
Sum of electronic and thermal Free Energies= -915.520703

Product (*OOH addition to C9)

\O,1.7501022404
,2.8784306736,0.0104053056\O,-2.5213675552,1.1390583998,-0.329550175\N
,2.3674365558,-2.5833951345,-0.1948564541\N,-3.2834109967,-0.990188091
3,-0.4452972961\C,0.2857143541,-1.9309158413,0.3044830822\C,1.10778620
56,-0.7855310478,0.1477938722\C,-1.1853317396,-1.8729781583,0.58249726
58\C,2.392442865,-1.2093506128,-0.1615643411\C,1.0971030329,-3.0264392
079,0.085490609\C,-1.9656478935,-1.5466697043,-0.7047230602\C,0.773548
0612,0.646477235,0.357161205\C,3.4623254482,-0.3152904745,-0.422138391
8\C,1.9096333549,1.5303437464,-0.0758349277\C,3.1685751253,1.056204647

7,-0.3845898438\C,-3.4480381761,0.3399964658,-0.2324442891\C,-4.845313
8295,0.7935433698,0.1277270182\C,0.4255080619,3.4039903965,-0.12709025
49\H,-1.5463368642,-2.8102611989,1.0135891388\H,-1.3737883631,-1.07860
61702,1.3089929098\H,0.8697990006,-4.0800234237,0.1155016418\H,-2.0776
940851,-2.4382985663,-1.3231948406\H,-1.4171781735,-0.80597073,-1.2849
44817\H,3.1554306946,-3.1736681646,-0.3960095997\H,-0.1740517102,0.917
8022806,-0.1186035906\H,4.4554889903,-0.6644201342,-0.6675799793\H,3.9
364314832,1.785921362,-0.6102393798\H,-4.0609129176,-1.6076380447,-0.2
834723134\H,-5.5841550992,-0.0071375743,0.0834745016\H,-5.1344364169,1
.5925546271,-0.5544433624\H,-4.822663399,1.2074006211,1.1365413599\H,0
.5421979562,4.4843513495,-0.1107208954\H,-0.0115972635,3.0942873225,-1
.0784658751\H,-0.2127601911,3.0821552675,0.6945799076\O,0.441665742,0.
9376946513,1.7517823488\O,1.5615505326,0.6095627561,2.5627076356\H,2.0
651783191,1.4398379773,2.5554551651\\

Zero-point correction= 0.298109 (Hartree/Particle)
Thermal correction to Energy= 0.317204
Thermal correction to Enthalpy= 0.318148
Thermal correction to Gibbs Free Energy= 0.249102
Sum of electronic and zero-point Energies= -915.500461
Sum of electronic and thermal Energies= -915.481366
Sum of electronic and thermal Enthalpies= -915.480421
Sum of electronic and thermal Free Energies= -915.549467

Product (*OOH addition to C10)

\O,2.1802463434
,-2.4180024981,-0.6247680611\O,-2.6166496395,-1.3621432101,-0.33275021
34\N,1.9386687766,2.8535896569,-0.0705482374\N,-3.5104889128,0.5410250
288,0.4934400055\C,-0.0890288695,1.918309338,-0.330177545\C,0.88834711
21,0.8726125641,-0.117576925\C,-1.5514793533,1.6776625697,-0.529642709
8\C,2.1393872055,1.505917557,0.0379553541\C,0.5939154753,3.1017743168,
-0.2925910148\C,-2.2080192338,1.135685472,0.7513854946\C,0.7714648268,
-0.5079061979,-0.0538996446\C,3.345541464,0.7687399625,0.2396090342\C,
1.9755471411,-1.3408450701,0.2444866904\C,3.2702824432,-0.5796633001,0
.305683977\C,-3.6085843334,-0.6960397425,-0.0543410637\C,-5.0074334455
,-1.2152796697,-0.3037550665\C,1.0273382963,-3.2081860774,-0.924755328
1\H,-2.0564902895,2.5931905366,-0.8483821923\H,-1.6891198879,0.9303227
699,-1.3156791865\H,0.235287128,4.1118338117,-0.412692881\H,-2.3331890
03,1.9333286692,1.4839774162\H,-1.5718981591,0.3701241701,1.1955206889
\H,2.655045203,3.5564866331,-0.0199441295\H,-0.1892381682,-1.000663262
3,-0.1336631507\H,4.3012130919,1.2762786637,0.3092632249\H,4.151910448
5,-1.1974326543,0.4229190117\H,-4.3480395072,1.0660629575,0.6766157022
\H,-5.7888820047,-0.529247172,0.0243494527\H,-5.118048252,-2.165717746
,0.2181015122\H,-5.1194491192,-1.406273487,-1.3713265063\H,1.408796143
,-4.1256894489,-1.3665205834\H,0.4648899479,-3.4401826382,-0.020293880
5\H,0.3840444845,-2.6966766718,-1.6429937964\O,1.789125025,-2.02360224
47,1.5382644624\O,1.4680815268,-1.0481401603,2.5174963801\H,2.34754200
58,-0.7445239962,2.7946593086\\

Zero-point correction= 0.296804 (Hartree/Particle)
Thermal correction to Energy= 0.316139
Thermal correction to Enthalpy= 0.317084
Thermal correction to Gibbs Free Energy= 0.247016
Sum of electronic and zero-point Energies= -915.491500
Sum of electronic and thermal Energies= -915.472164
Sum of electronic and thermal Enthalpies= -915.471220
Sum of electronic and thermal Free Energies= -915.541287

Product (*OOH addition to C11)

\O,-1.756596629
3,2.7134918422,-0.2963697062\O,2.726711541,1.2981850651,-0.245819652\N
,-2.0150799546,-2.782237059,-0.1183145902\N,3.4886172923,-0.6310432121
,0.6523805872\C,0.0601563041,-1.9208630047,-0.2912758792\C,-0.86365379
66,-0.8488992256,-0.2238406303\C,1.5442003778,-1.7581655969,-0.4147282

292\C,-2.1724304733,-1.4036919503,-0.1137540214\C,-0.6776739634,-3.088
0087025,-0.2232344432\C,2.1496470588,-1.1587982584,0.864949533\C,-0.67
56901374,0.56763742,-0.306138026\C,-3.3065676374,-0.6338828482,-0.0626
847237\C,-1.767202857,1.3670327794,-0.2237334935\C,-3.1686326784,0.854
0965306,0.0004221274\C,3.6710415492,0.586211614,0.0825969727\C,5.10328
95942,1.026528278,-0.1242647012\C,-0.4814900147,3.3373328194,-0.379333
8339\H,2.0231244796,-2.713987257,-0.6426327362\H,1.7647690282,-1.07461
44752,-1.2392750606\H,-0.3445853892,-4.113477039,-0.249844937\H,2.1951
701844,-1.9083657391,1.6556487019\H,1.5242749673,-0.338030753,1.215751
9933\H,-2.762574298,-3.4508866453,-0.0715314579\H,0.3227271998,0.96526
40031,-0.4371240819\H,-4.3046574998,-1.0520779569,-0.0277754965\H,-3.8
447720353,1.3541259469,-0.7012032815\H,4.2912341669,-1.1972721703,0.86
76965526\H,5.834886194,0.3067689105,0.243885852\H,5.2461140001,1.97958
87687,0.3849036147\H,5.2630044516,1.1911075175,-1.1901339138\H,-0.6732
92752,4.4065627928,-0.3804505408\H,0.1330883322,3.0627088592,0.4800841
335\H,0.0319224957,3.0457737145,-1.2983766952\O,-3.6878202548,1.367037
292,1.2591148581\O,-2.8316388464,0.9284223761,2.3045763058\H,-3.123385
3895,0.0115405634,2.4366073993\

Zero-point correction= 0.297798 (Hartree/Particle)
Thermal correction to Energy= 0.316916
Thermal correction to Enthalpy= 0.317860
Thermal correction to Gibbs Free Energy= 0.248766
Sum of electronic and zero-point Energies= -915.496013
Sum of electronic and thermal Energies= -915.476895
Sum of electronic and thermal Enthalpies= -915.475951
Sum of electronic and thermal Free Energies= -915.545045

Product (*OOH addition to C12)

\O,-1.310926960
6,3.0704151638,-0.0220960163\O,2.8485568635,1.0586218474,-0.0548416761
\N,-2.3233140746,-2.3285641385,-0.3036432774\N,3.3781842619,-1.0329467
017,0.6193625127\C,-0.156134937,-1.7935184669,-0.4696516924\C,-0.93560
82941,-0.5923036336,-0.3451731096\C,1.337244231,-1.8192447087,-0.57293
06288\C,-2.2642080044,-0.9718182659,-0.2453813385\C,-1.0463432444,-2.8
376558673,-0.4286697548\C,1.9852396913,-1.4275069333,0.765648231\C,-0.
5510737164,0.7741041559,-0.2773096748\C,-3.3978245536,-0.0340161797,-0
.0561443886\C,-1.5814980594,1.7324515446,-0.1003650238\C,-2.9066763034
,1.3788957746,-0.0091165184\C,3.7031985849,0.2118319393,0.1934762368\C
,5.1777392118,0.5102989635,0.0391662195\C,0.0426751163,3.4816307976,-0
.1601743208\H,1.6931037644,-2.8033550883,-0.8881217525\H,1.6611115408,
-1.0945309847,-1.3248521138\H,-0.8773092148,-3.9008511367,-0.488693475
2\H,1.9300531813,-2.2532782578,1.4752953699\H,1.4498588762,-0.58086560
43,1.1946688033\H,-3.157187406,-2.8705898747,-0.1513657895\H,0.4917054
351,1.0508419445,-0.3408139534\H,-4.1663888359,-0.1550717723,-0.830641
6839\H,-3.6473559485,2.1628990862,0.0873606656\H,4.1094531975,-1.70615
5637,0.7722639329\H,5.8205917285,-0.3186309282,0.3363067578\H,5.415428
4979,1.3866885414,0.6419717523\H,5.3714274015,0.7613038748,-1.00409537
88\H,0.0277715594,4.5649840569,-0.0736008178\H,0.6706695714,3.05615676
47,0.6254075968\H,0.4436231573,3.1953492171,-1.1351742038\O,-4.1802495
064,-0.3781403281,1.1218200405\O,-3.3138284635,-0.3709362778,2.2484565
394\H,-3.2004695288,0.5809253733,2.4108687604\

Zero-point correction= 0.297768 (Hartree/Particle)
Thermal correction to Energy= 0.317004
Thermal correction to Enthalpy= 0.317948
Thermal correction to Gibbs Free Energy= 0.247464
Sum of electronic and zero-point Energies= -915.498476
Sum of electronic and thermal Energies= -915.479240
Sum of electronic and thermal Enthalpies= -915.478296
Sum of electronic and thermal Free Energies= -915.548781

Product (*OO-CH=CH₂ addition to C5)

\O,-0.8810022771,3.467516934,0.284

5783119\O,2.8291889965,1.1391665986,-0.2886734299\N,-2.6677019364,-1.6
842891196,-0.5152767163\N,3.3058052002,-1.0500049065,0.0223795279\C,-0
.4750662151,-1.5761061624,0.3068967548\C,-1.0766810264,-0.1939105445,0
.1475432942\C,0.9462880252,-1.7591402921,-0.2461088554\C,-2.3844961984
,-0.3278335351,-0.3160204742\C,-1.5167434266,-2.4214097832,-0.34382794
38\C,2.060007506,-1.322495403,0.7222421321\C,-0.5208758973,1.061110442
4,0.367967979\C,-3.1883622556,0.7847792558,-0.5412896729\C,-1.31637338
2,2.1843260167,0.1279573231\C,-2.6399753253,2.0401735829,-0.30946881\C
,3.5870585495,0.188186125,-0.4542560827\C,4.8938231221,0.3402913773,-1
.2007732207\C,0.4742634971,3.648453408,0.6719110948\H,1.0910717119,-2.
8082815644,-0.5190644829\H,1.0157977584,-1.1647885432,-1.1586561399\H,
-1.5320806249,-3.499029366,-0.3591869954\H,2.243696288,-2.0912619412,1
.4705105283\H,1.7851912022,-0.4138748426,1.2502656899\H,-3.4502813826,
-2.0045705174,-1.0594783336\H,0.5105893946,1.1630965567,0.6711400391\H
,-4.2071108665,0.6865402423,-0.8962221152\H,-3.2196395107,2.9385379713
,-0.4783256503\H,3.9451973632,-1.8033721504,-0.1657855242\H,5.48383163
91,-0.5760520428,-1.2319379132\H,5.4739151231,1.1283105286,-0.72083705
89\H,4.6728972322,0.6620684992,-2.2188598475\H,0.631601202,4.723539507
7,0.696541781\H,0.6515292677,3.2298269767,1.6663560732\H,1.1560348288,
3.1846102574,-0.0433196568\O,-0.2960601585,-1.9309652226,1.7334738617\O,
-1.5428830477,-1.7790896788,2.3953953489\C,-2.0697168192,-3.02135822
67,2.633194947\H,-1.3313764739,-3.8127013251,2.6672444626\C,-3.3688588
843,-3.1735226418,2.8693758171\H,-3.7510982571,-4.145063316,3.14755361
6\H,-4.049473712,-2.3345579851,2.8103640915\

Zero-point correction= 0.330527 (Hartree/Particle)
Thermal correction to Energy= 0.352026
Thermal correction to Enthalpy= 0.352971
Thermal correction to Gibbs Free Energy= 0.278040
Sum of electronic and zero-point Energies= -992.842665
Sum of electronic and thermal Energies= -992.821166
Sum of electronic and thermal Enthalpies= -992.820222
Sum of electronic and thermal Free Energies= -992.895152

Product (*OO-CH=CH₂ addition to C6)

\O,0.6214140558
,3.501760141,0.5879364131\O,-3.1843395674,0.7946373048,0.0596766438\N,
2.6615226107,-1.5546644251,-0.3392576148\N,-3.3402731657,-1.1786446952
,-1.0317114201\C,0.341931515,-1.3863227912,-0.2283124922\C,0.890685681
1,-0.1141032638,-0.0340495575\C,-1.096288833,-1.7473458208,-0.11241886
56\C,2.3014181052,-0.214334505,-0.1472418438\C,1.4605004994,-2.3481088
998,-0.5038503033\C,-1.9144600182,-1.2264599614,-1.3120849106\C,0.2714
175498,1.1279135902,0.2355547154\C,3.1040820201,0.9076981226,-0.027024
7204\C,1.0862835871,2.2422830535,0.3482385496\C,2.4872816199,2.1364881
172,0.2126847011\C,-3.8678805928,-0.1523856529,-0.3181736674\C,-5.3460
580902,-0.2356756999,-0.0105167127\C,-0.7851021249,3.6516953552,0.7128
779246\H,-1.2144604173,-2.8286657346,-0.0094263142\H,-1.5058544863,-1.
282804024,0.7902220995\H,-1.7568405944,-1.8521976641,-2.1911508269\H,-
1.5969569329,-0.2129773728,-1.5548383426\H,3.4379618161,-1.7553866141,
-0.9501075584\H,-0.8056318296,1.1810641943,0.3275688419\H,4.1825557875
,0.8426086307,-0.103180479\H,3.0731763097,3.0406676158,0.3112157906\H,
-3.9219669791,-1.9665779549,-1.2609410652\H,-5.8456746193,-1.063193518
8,-0.5147356234\H,-5.8117182142,0.7042854918,-0.304975882\H,-5.4681846
,-0.345347562,1.0678442176\H,-0.9555302328,4.7102776146,0.8900549715\H
,-1.2952275609,3.3387324983,-0.2010631668\H,-1.167182372,3.0675735064,
1.5535159599\H,1.4074325967,-2.8299733768,-1.4890136974\O,1.4378777313
,-3.5115541019,0.338162141\O,1.3138544072,-3.0621815498,1.6875281093\C
,2.4762393611,-3.368632147,2.3501894312\H,3.358299102,-3.3515177364,1.
7248859969\C,2.4588731096,-3.5884526979,3.6597339956\H,1.5302397651,-3.
.5956464899,4.2146600256\H,3.3892839106,-3.7319266466,4.1895951562\

Zero-point correction= 0.331469 (Hartree/Particle)
Thermal correction to Energy= 0.352543
Thermal correction to Enthalpy= 0.353488

Thermal correction to Gibbs Free Energy= 0.278887
Sum of electronic and zero-point Energies= -992.860831
Sum of electronic and thermal Energies= -992.839757
Sum of electronic and thermal Enthalpies= -992.838813
Sum of electronic and thermal Free Energies= -992.913414

Product (*OO-CH=CH₂ addition to C7)

\O,-1.194601519

2,3.0306804066,0.2332661714\O,3.0014963426,0.9946373545,-0.0101921792\
N,-2.3254539286,-2.2247748042,-0.744701188\N,3.5269586629,-1.185258309
1,0.280286921\C,-0.0907059191,-1.7227373499,-0.6554433454\C,-0.8127851
496,-0.5759349828,-0.1923856443\C,1.3899493667,-1.7365394303,-0.870352
2563\C,-2.2236003005,-1.0087761679,0.0260554912\C,-1.0171647633,-2.681
8398094,-0.942109829\C,2.1404511536,-1.5878255187,0.4630996458\C,-0.42
38995554,0.7466990444,-0.0496692175\C,-3.2185502456,0.0704085206,-0.16
7223533\C,-1.4262198654,1.7076241252,0.0746329366\C,-2.8145864883,1.35
80237907,-0.0610671235\C,3.850316577,0.1082551668,0.0391128474\C,5.318
2756675,0.4096185357,-0.1668165629\C,0.1630141386,3.4407083559,0.36194
64405\H,1.703234489,-2.6510013149,-1.3801681976\H,1.6683531587,-0.8903
134238,-1.5062341194\H,-0.8533824903,-3.6632041119,-1.3630469825\H,2.1
235502245,-2.5247369835,1.0198340384\H,1.6537402746,-0.8279835138,1.07
39369756\H,-3.0167814781,-2.8904078406,-0.4273543854\H,0.6235815146,1.
0140096799,-0.1155551525\H,-4.2611527844,-0.1929863496,-0.2947862415\H
,-3.5234841389,2.1760046087,-0.0975454582\H,4.2529302184,-1.8809923169
,0.2726974554\H,5.4507417612,0.8092178318,-1.1727333917\H,5.9614254041
,-0.4611432664,-0.037054286\H,5.6115830281,1.1849430599,0.540717112\H,
0.1313450304,4.5107180267,0.5472852143\H,0.6421632269,2.9254823808,1.1
965390083\H,0.7191651959,3.2359719702,-0.5547610192\O,-2.3654902114,-1.
.560500737,1.4336807784\O,-2.0394473686,-0.5430893052,2.3641194416\C,-
3.1782001452,-0.1255257776,3.000580961\H,-4.0383016742,-0.7568391083,2
.8194837255\C,-3.1628133249,0.9394981743,3.7953185649\H,-2.2678069994,
1.5334581655,3.9241690365\H,-4.0608814749,1.2195471736,4.3259570371\

Zero-point correction= 0.330066 (Hartree/Particle)

Thermal correction to Energy= 0.351242
Thermal correction to Enthalpy= 0.352186
Thermal correction to Gibbs Free Energy= 0.278161
Sum of electronic and zero-point Energies= -992.833085
Sum of electronic and thermal Energies= -992.811909
Sum of electronic and thermal Enthalpies= -992.810965
Sum of electronic and thermal Free Energies= -992.884990

Product (*OO-CH=CH₂ addition to C8)

\O,-1.519210947

2,3.1260966241,0.1042531962\O,2.913858564,1.3224519362,-0.3792501351\N
,-2.2586093513,-2.224468109,-0.3136657916\N,3.5889118529,-0.7853599495
,0.0801600686\C,-0.0773739058,-1.5952061501,-0.4463680472\C,-0.8309209
422,-0.518017581,0.289190254\C,1.3781210133,-1.5020552415,-0.769808309
5\C,-2.2578584331,-0.9285386255,0.1188738515\C,-0.9564315608,-2.572628
2897,-0.7199998129\C,2.2519900252,-1.2179903573,0.4622422838\C,-0.5738
394254,0.9141959044,0.0144455944\C,-3.2922759354,-0.0297109279,0.33305
23544\C,-1.6142978799,1.7727398574,0.1841823792\C,-2.9632078592,1.3154
179203,0.4269530758\C,3.8130468537,0.4876408803,-0.3260109256\C,5.2352
807019,0.8334051835,-0.7096523866\C,-0.2179158957,3.6556136408,-0.1117
026512\H,1.7154120844,-2.4160297445,-1.266652163\H,1.528098302,-0.6738
763458,-1.4703130851\H,-0.787922446,-3.5285554875,-1.193382652\H,2.336
1731286,-2.1036728812,1.0919264721\H,1.8066146018,-0.4283515922,1.0629
817498\H,-3.0842074876,-2.7125311839,-0.6146911627\H,0.4434384733,1.22
79634176,-0.1778577846\H,-4.3267494566,-0.3505234053,0.3590922223\H,-3
.7201863128,2.0700336644,0.5868943832\H,4.3486336785,-1.4438876026,0.0
75865958\H,5.242141704,1.166281363,-1.747794467\H,5.9296546024,0.00100
96222,-0.5921295624\H,5.5638002303,1.6678499786,-0.0898758492\H,-0.331
1843684,4.736228909,-0.1052655568\H,0.4625521385,3.34117578,0.68266499

95\H,0.1781225047,3.3264181474,-1.0749836851\O,-0.4925382323,-0.593086
3012,1.7706387445\O,-0.7369046047,-1.9120916352,2.2612507202\C,-1.8901
834658,-1.8958513867,2.9960832131\H,-2.2121778655,-0.9028567264,3.2835
663005\C,-2.4988218232,-3.0282446683,3.3389536945\H,-2.1263654746,-3.9
897788848,3.010958218\H,-3.369235836,-2.9915250022,3.977772834\
Zero-point correction= 0.329898 (Hartree/Particle)
Thermal correction to Energy= 0.351261
Thermal correction to Enthalpy= 0.352205
Thermal correction to Gibbs Free Energy= 0.277998
Sum of electronic and zero-point Energies= -992.824106
Sum of electronic and thermal Energies= -992.802743
Sum of electronic and thermal Enthalpies= -992.801798
Sum of electronic and thermal Free Energies= -992.876006

Product (*OO-CH=CH₂ addition to C9)

\O,-1.672852274,-2.1160619983,-1.5380732974\O,2.7185794139,-1.
3625442593,-0.5009157464\N,-1.3160060687,3.228845691,-0.2966867078\N,3
.8564775541,0.4874258129,0.1377373307\C,0.4291609643,2.0209377049,0.41
30123123\C,-0.5100921503,1.1612642167,-0.2129105329\C,1.753365982,1.56
7055164,0.9473153408\C,-1.5830603538,1.9267109175,-0.6461021162\C,-0.1
015243767,3.2935165605,0.3435580009\C,2.7657114893,1.3873736782,-0.200
1355361\C,-0.4945653884,-0.3172818835,-0.3397174204\C,-2.6866600655,1.
3842803697,-1.3540103255\C,-1.5980958303,-0.7913991912,-1.2397069642\C
,-2.6421137764,0.0145346581,-1.6482837343\C,3.724443218,-0.8542594529,
-0.0136384299\C,4.8913027331,-1.7004752114,0.4438430157\C,-0.461240834
8,-2.8770216258,-1.5126153635\H,2.1454822775,2.2681796796,1.6883178292
\H,1.6219771887,0.601465915,1.4417894445\H,0.287830126,4.2323227371,0.
7038185407\H,3.18576673,2.3493010834,-0.4970851153\H,2.2607644392,0.96
28270632,-1.0667081883\H,-1.9145943353,4.0142885796,-0.4831333993\H,0.
4876900426,-0.6908592648,-0.6429707513\H,-3.5154128509,1.9965194598,-1
.6806841768\H,-3.4361045206,-0.4474962015,-2.2215303841\H,4.673935097,
0.8462086248,0.6009309781\H,5.7382155777,-1.1130187218,0.7994225349\H,
5.2094581275,-2.3269475233,-0.389272656\H,4.5466000173,-2.3573242725,1
.2430794861\H,-0.7387639055,-3.8704942667,-1.8546852812\H,0.2780617619
,-2.4460027151,-2.1904319511\H,-0.0489701195,-2.9287436053,-0.50510537
58\O,-0.6050703947,-0.979040218,0.9674090473\O,-1.8056169899,-0.524185
3938,1.5881080317\C,-2.6802668256,-1.576767057,1.6563630058\H,-2.53625
64584,-2.3278021642,0.8897219946\C,-3.6419616625,-1.5925319904,2.57368
43497\H,-3.7203750727,-0.8116220005,3.318341546\H,-4.3753412975,-2.385
6691212,2.5626726717\
Zero-point correction= 0.331386 (Hartree/Particle)
Thermal correction to Energy= 0.352751
Thermal correction to Enthalpy= 0.353695
Thermal correction to Gibbs Free Energy= 0.278280
Sum of electronic and zero-point Energies= -992.850874
Sum of electronic and thermal Energies= -992.829509
Sum of electronic and thermal Enthalpies= -992.828565
Sum of electronic and thermal Free Energies= -992.903980

Product (*OO-CH=CH₂ addition to C10)

\O,2.0002598545
,-2.4244223801,-0.9888323159\O,-2.7387265058,-1.288912221,-0.495239743
9\N,1.8861649323,2.7924492136,0.1370416538\N,-3.578078645,0.513873876,
0.5770238921\C,-0.1646919477,1.9348069163,-0.1970064654\C,0.7963372219
,0.85453459,-0.1457031453\C,-1.6368502637,1.7424147495,-0.3778879171\C
,2.0623271856,1.4398265374,0.0661751569\C,0.541945292,3.0909908437,-0.
0171430839\C,-2.2597537384,1.0636407426,0.8538714595\C,0.6538514277,-0.
.5203907569,-0.2594384289\C,3.2573983129,0.6626766593,0.1370497775\C,1
.8413795115,-1.3995943997,-0.0540120882\C,3.1537590955,-0.6807743494,0
.0459364548\C,-3.7114111697,-0.652839514,-0.1016363893\C,-5.12459865,-
1.1342950157,-0.3456480996\C,0.8142485381,-3.1336937248,-1.3553275082\
H,-2.1341606605,2.6965674676,-0.5703844271\H,-1.8134834472,1.094300473

9,-1.2404414976\H,0.2008471319,4.1137917676,0.009936308\H,-2.349771094
,1.7737015609,1.6764448796\H,-1.6190282894,0.2465051383,1.1858914643\H
,2.6149984523,3.4680199803,0.286713869\H,-0.3176219898,-0.9811433993,-
0.3845919736\H,4.2245112551,1.1395686488,0.2462681212\H,4.0234282466,-
1.3250235303,0.0720049158\H,-4.4018429695,1.0202105323,0.8521698571\H,
-5.8846785124,-0.4768889642,0.0774996425\H,-5.2260915676,-2.1295071131
,0.0873926904\H,-5.2795332226,-1.2214467501,-1.4212409522\H,1.15672598
32,-4.0340595897,-1.8595477852\H,0.2302774094,-3.4029987027,-0.4749869
104\H,0.2055200085,-2.5398243491,-2.039084325\O,1.6458186112,-2.184667
8127,1.1998846818\O,1.3347156209,-1.2742325559,2.2430946561\C,2.396641
5305,-1.1997870329,3.1031436485\H,3.1839730156,-1.9099683689,2.8878161
744\C,2.3955030512,-0.3395371568,4.1169737125\H,1.5733879343,0.3456200
192,4.2753044602\H,3.2296131204,-0.32785668,4.8029926607\H
Zero-point correction= 0.329796 (Hartree/Particle)
Thermal correction to Energy= 0.351348
Thermal correction to Enthalpy= 0.352292
Thermal correction to Gibbs Free Energy= 0.275811
Sum of electronic and zero-point Energies= -992.841826
Sum of electronic and thermal Energies= -992.820274
Sum of electronic and thermal Enthalpies= -992.819330
Sum of electronic and thermal Free Energies= -992.895810

Product (*OO-CH=CH₂ addition to C11)

\O,1.6270137566,-2.7310241068,-0.8
46663273\O,-2.8519031636,-1.3216408279,-0.3174562101\N,1.9441658992,2.
6891723436,0.0370411698\N,-3.4979494688,0.4423908919,0.939716229\C,-0.
1481829881,1.8630913734,-0.0910259029\C,0.7660134049,0.793402554,-0.25
60344697\C,-1.6388117175,1.7193481143,-0.1143222851\C,2.083358031,1.32
45749612,-0.1611268031\C,0.6079459135,3.0056315787,0.0988510562\C,-2.1
371846999,0.9292974371,1.1069906842\C,0.5573356115,-0.5981254546,-0.52
74857524\C,3.2099640894,0.5510625676,-0.2774292893\C,1.6439362047,-1.4
043938258,-0.5899020722\C,3.0457082844,-0.9281663326,-0.3106191249\C,-
3.7505819882,-0.6698861338,0.2061154538\C,-5.2024558522,-1.0718587426,
0.0684921891\C,0.3472527078,-3.3328316424,-0.9929009288\H,-2.124680036
8,2.6978453868,-0.1500283381\H,-1.9378777464,1.1701182235,-1.011285843
8\H,0.2864190989,4.0226457463,0.2595480579\H,-2.0994926118,1.547444300
4,2.0044469169\H,-1.4951981449,0.0635621266,1.2679070779\H,2.699447879
4,3.3212000543,0.2334755386\H,-0.4489399586,-0.968908704,-0.676131697\
H,4.211992688,0.955651998,-0.222738393\H,3.7337735716,-1.4113151454,-1.
.0102076588\H,-4.2684517289,0.9683217389,1.3150412843\H,-5.8852290816,
-0.4226830214,0.6172602116\H,-5.3101367525,-2.095487528,0.4269546235\H
,-5.4649575103,-1.0600109602,-0.9896649107\H,0.5320376241,-4.391795139
,-1.1491963007\H,-0.251655026,-3.1803976978,-0.092852916\H,-0.17998229
47,-2.9121619468,-1.8522343177\O,3.5164793552,-1.5382352845,0.94226483
43\O,2.6778483386,-1.0645871216,1.9910581046\C,3.3689069798,-0.1366043
77,2.7213975367\H,4.4442816798,-0.2595636664,2.684072507\C,2.725406252
5,0.7668044541,3.4552129867\H,1.646034224,0.8426444789,3.4261573227\H,
3.2838830759,1.4258970288,4.1043067027\H
Zero-point correction= 0.331328 (Hartree/Particle)
Thermal correction to Energy= 0.352638
Thermal correction to Enthalpy= 0.353582
Thermal correction to Gibbs Free Energy= 0.278492
Sum of electronic and zero-point Energies= -992.846567
Sum of electronic and thermal Energies= -992.825257
Sum of electronic and thermal Enthalpies= -992.824312
Sum of electronic and thermal Free Energies= -992.899403

Product (*OO-CH=CH₂ addition to C12)

\O,-1.221605597
6,3.0163571131,-0.082782185\O,2.9813437247,1.0504805225,0.0969092394\N
,-2.1237894684,-2.3754880263,-0.7022855104\N,3.4835577108,-1.071415933
4,0.6939875899\C,0.0407564868,-1.8066245912,-0.6738413074\C,-0.7630770

503,-0.6238442555,-0.5370236964\C,1.5379108135,-1.8131314011,-0.672326
8182\C,-2.0891220663,-1.0222625557,-0.5617680472\C,-0.8342503667,-2.86
1382156,-0.7611273278\C,2.0884123669,-1.4832299879,0.7254180911\C,-0.4
066106245,0.7434042115,-0.3718926026\C,-3.2442810549,-0.1084992882,-0.
3960971858\C,-1.460853927,1.678757057,-0.236604062\C,-2.783593953,1.30
53905481,-0.2682797225\C,3.8246465894,0.1960810998,0.3563396591\C,5.30
36459146,0.510483039,0.3201172111\C,0.1325900601,3.4456774174,-0.04663
34229\H,1.9254583312,-2.778069441,-1.0088193602\H,1.905605102,-1.05076
20148,-1.3646357704\H,-0.6447539852,-3.9170214029,-0.8719598568\H,1.99
57689886,-2.3446904593,1.3871057792\H,1.5153523091,-0.6644307929,1.159
5173033\H,-2.9582512746,-2.9356666841,-0.6545368027\H,0.633018287,1.03
59871342,-0.3390367986\H,-3.9746376125,-0.2135393568,-1.2087553745\H,-
3.5401042865,2.0753683946,-0.1894702312\H,4.2097476225,-1.7475569024,0
.8573045059\H,5.932359558,-0.3310242248,0.6121785913\H,5.4917607576,1.
3512762826,0.9876708043\H,5.5653921002,0.8230920555,-0.691083308\H,0.0
929252333,4.5230042528,0.09235364\H,0.6733060648,2.9850858989,0.782823
3218\H,0.6454384268,3.2142186134,-0.9830844896\O,-4.0910576259,-0.5325
479568,0.7203382001\O,-3.2694333919,-0.5926910714,1.8832369354\C,-3.68
5124175,-3.4053932351,0.2735673269,4.0557841175\H,-2.8924216407,-0.591
3261204,4.4546476075\H,-3.6714855112,1.0812975449,4.7216359278\\
Zero-point correction= 0.330706 (Hartree/Particle)
Thermal correction to Energy= 0.352291
Thermal correction to Enthalpy= 0.353235
Thermal correction to Gibbs Free Energy= 0.275913
Sum of electronic and zero-point Energies= -992.847423
Sum of electronic and thermal Energies= -992.825838
Sum of electronic and thermal Enthalpies= -992.824894
Sum of electronic and thermal Free Energies= -992.902216

Product (*OO-CH₂-CH=CH₂ addition to C5)

\O,-0.9249518373,3.4407787762,0.19
61146284\O,2.8296391503,1.1880476383,-0.3790790387\N,-2.6255688408,-1.
7778982855,-0.3603436575\N,3.347587099,-0.9868709149,-0.0301110358\C,-
0.4071577486,-1.5898753167,0.4076862735\C,-1.0450995266,-0.226954528,0
.2064327208\C,0.9978115856,-1.7599452287,-0.1918500009\C,-2.3568453053
,-0.4058932952,-0.2267125262\C,-1.4456673915,-2.4782250926,-0.19515113
06\C,2.1316303612,-1.2613375246,0.7205295737\C,-0.5132462856,1.0469912
615,0.3684806238\C,-3.1874800065,0.6795030328,-0.4814700558\C,-1.33589
65846,2.1433852022,0.0972590008\C,-2.6626001145,1.9550279723,-0.311736
0261\C,3.5917401132,0.2414573883,-0.5503150077\C,4.8647166961,0.389139
7205,-1.3544507703\C,0.4326329785,3.6643190354,0.5511294884\H,1.159581
484,-2.8152335511,-0.4302951033\H,1.0211518326,-1.1998905688,-1.128254
0018\H,-1.4285157508,-3.5564404713,-0.1860203707\H,2.3572952533,-1.996
3877938,1.4909138533\H,1.8525486525,-0.3396529181,1.222663378\H,-3.360
5518578,-2.1096037805,-0.9633548545\H,0.5201681564,1.1820696563,0.6513
268196\H,-4.211125141,0.5454116997,-0.8097670021\H,-3.2641632897,2.833
5911071,-0.5063212725\H,3.9860790208,-1.7377224782,-0.2312073438\H,5.4
685823862,-0.518341016,-1.3798621568\H,5.4501849635,1.2018142892,-0.92
48736811\H,4.5973051377,0.6730844762,-2.3726790836\H,0.5682177516,4.74
25078117,0.529454636\H,0.6358011727,3.2902229339,1.5583303604\H,1.1115
335147,3.1853677541,-0.15679938\O,-0.1830513929,-1.8829262363,1.828005
1147\O,-1.4095938521,-1.6721220135,2.5201005453\C,-1.7662189277,-2.922
1506599,3.104026073\H,-2.0240172921,-3.6434856113,2.3240332257\H,-0.90
96452122,-3.2946576713,3.6738518422\C,-2.9335781043,-2.6541300641,4.00
29968751\H,-2.7822608251,-1.9000106097,4.7687600265\C,-4.0942399948,-3
.296951523,3.9013800244\H,-4.2601763271,-4.0410779457,3.1297335648\H,-
4.9115687909,-3.1014901168,4.5843371313\\
Zero-point correction= 0.360115 (Hartree/Particle)
Thermal correction to Energy= 0.382903
Thermal correction to Enthalpy= 0.383847
Thermal correction to Gibbs Free Energy= 0.305426

Sum of electronic and zero-point Energies= -1032.116566
Sum of electronic and thermal Energies= -1032.093779
Sum of electronic and thermal Enthalpies= -1032.092834
Sum of electronic and thermal Free Energies= -1032.171255

Product (*OO-CH₂-CH=CH₂ addition to C6)

\O,0.6156586293
,3.4323605554,0.7362550847\O,-3.2058452897,0.7836449171,0.031776672\N,
2.6261609229,-1.6248094344,-0.2507984969\N,-3.3519483688,-1.1646007513
,-1.1056816373\C,0.305759505,-1.4315442891,-0.2125383602\C,0.86204502,
-0.1702668628,0.0252796872\C,-1.1387415051,-1.7779366106,-0.1412613972
\C,2.2746465772,-0.2852739403,-0.0460880692\C,1.4208598558,-2.40713294
88,-0.4624340841\C,-1.9196935801,-1.22134794,-1.3495722405\C,0.2497810
387,1.0725813845,0.3084511721\C,3.0855113462,0.8244456792,0.1250057256
\C,1.0736704359,2.1740118494,0.4742665984\C,2.4761969084,2.0552744984,
0.3763706142\C,-3.8877628275,-0.1489106698,-0.3832608971\C,-5.37446705
44,-0.223825182,-0.116346387\C,-0.7906056842,3.589016209,0.855457189\H
,-1.2702762933,-2.8598970591,-0.0657635378\H,-1.5661555451,-1.32969271
41,0.7614979753\H,-1.7454669589,-1.8293687986,-2.2378769101\H,-1.58657
85963,-0.205950055,-1.5618688557\H,3.4192499683,-1.8249739407,-0.84009
23548\H,-0.8288592541,1.1367285808,0.3702867872\H,4.1650623761,0.74803
92135,0.0791615626\H,3.0691955854,2.9496615257,0.5143112862\H,-3.93411
07683,-1.9437748426,-1.3618320389\H,-5.8642456636,-1.05027272,-0.63190
70722\H,-5.8273223814,0.717274338,-0.4268892355\H,-5.5269052912,-0.329
2466524,0.9584846431\H,-0.9545494248,4.6424968275,1.0664965757\H,-1.29
72269897,3.3106380074,-0.0716343284\H,-1.1831534389,2.9800257346,1.673
5550626\H,1.3951940519,-2.8683486245,-1.4582420769\O,1.3522927253,-3.5
718702772,0.3656370088\O,1.2095963189,-3.1255266065,1.7128000773\C,2.4
082574723,-3.489722639,2.4030807309\H,2.463917161,-4.5773803518,2.4986
147976\H,3.2584566784,-3.1210042718,1.8264388893\C,2.3378936492,-2.823
3316435,3.74233179\H,2.2411202703,-1.7420199495,3.7289850831\C,2.40905
31639,-3.4882886633,4.8928752015\H,2.4942131746,-4.5695474616,4.913889
6599\H,2.3881027807,-2.9747498902,5.8460658155\

Zero-point correction= 0.360987 (Hartree/Particle)
Thermal correction to Energy= 0.383377
Thermal correction to Enthalpy= 0.384321
Thermal correction to Gibbs Free Energy= 0.305793
Sum of electronic and zero-point Energies= -1032.136933
Sum of electronic and thermal Energies= -1032.114543
Sum of electronic and thermal Enthalpies= -1032.113599
Sum of electronic and thermal Free Energies= -1032.192126

Product (*OO-CH₂-CH=CH₂ addition to C7)

\O,-1.184799595
2,2.9598414617,0.530958197\O,3.0300450609,0.9720942246,0.0306052481\N,
-2.2998769293,-2.2293637133,-0.7967366174\N,3.5710044238,-1.2203405889
,0.139451024\C,-0.0673559092,-1.7055871991,-0.7415367552\C,-0.78455501
54,-0.6015364995,-0.179247611\C,1.4068982256,-1.6916691546,-0.99681582
74\C,-2.1852533631,-1.0669007262,0.0571222629\C,-0.992966992,-2.653684
017,-1.0646479777\C,2.1906610508,-1.6429147704,0.3247240981\C,-0.40275
19809,0.7121880311,0.0427561436\C,-3.1918606053,0.0168524414,-0.058385
7987\C,-1.4089268558,1.6500337734,0.2671214028\C,-2.7972927104,1.29835
48861,0.1327087617\C,3.8835025364,0.089820371,-0.0087195676\C,5.345860
0508,0.4149838874,-0.2191017198\C,0.1738120002,3.3740960282,0.63509306
13\H,1.7108809884,-2.5614531447,-1.5846512543\H,1.6647222363,-0.796406
0773,-1.5714433884\H,-0.8309462858,-3.6020157422,-1.5563267418\H,2.190
5255965,-2.6205427384,0.8070486023\H,1.7168467602,-0.9355749521,1.0049
380741\H,-2.962582746,-2.9273281837,-0.4866717673\H,0.6403256848,0.993
9268398,-0.0316906566\H,-4.2323250483,-0.2468407161,-0.2037241795\H,-3
.5120262491,2.1128503287,0.1490364476\H,4.298848878,-1.9096694838,0.05
98068499\H,5.4514316802,0.930062583,-1.1741267441\H,5.9903361924,-0.46
43701164,-0.2092933419\H,5.6605270419,1.1018945587,0.5666067197\H,0.14

19021217,4.4262747582,0.9039608144\H,0.6925890141,2.8013380707,1.40614
27167\H,0.6915904387,3.246843674,-0.3175614309\O,-2.2835694127,-1.6901
334073,1.4196743652\O,-1.933036177,-0.705922982,2.381556156\C,-3.08776
41659,-0.4567712152,3.1814612864\H,-3.9435837745,-0.3078025341,2.51827
62628\H,-3.2804277513,-1.3098018234,3.8383987632\C,-2.7997833511,0.788
5024925,3.9617416009\H,-2.5436363161,1.6636453807,3.371007476\C,-2.863
6532987,0.8530901776,5.2894046149\H,-3.1049157752,-0.0209270988,5.8850
952578\H,-2.6804154735,1.778845786,5.8207635182\

Zero-point correction= 0.359807 (Hartree/Particle)
Thermal correction to Energy= 0.382169
Thermal correction to Enthalpy= 0.383114
Thermal correction to Gibbs Free Energy= 0.305914
Sum of electronic and zero-point Energies= -1032.108510
Sum of electronic and thermal Energies= -1032.086147
Sum of electronic and thermal Enthalpies= -1032.085203
Sum of electronic and thermal Free Energies= -1032.162403

Product (*OO-CH₂-CH=CH₂ addition to C8)

\O,-1.5436671715,3.1655821815,0.02
94091314\O,2.9405667486,1.3032293884,-0.4507989634\N,-2.2884610259,-2.
2095559012,-0.103219583\N,3.5811751108,-0.8106031184,0.0329430065\C,-0
.1140650209,-1.5663621525,-0.3622094986\C,-0.8337518102,-0.4708512435,
0.3889253659\C,1.3298705376,-1.4892206934,-0.7361401259\C,-2.268195972
3,-0.8880797407,0.2707148361\C,-0.9999478864,-2.5489680526,-0.57682313
76\C,2.2472319991,-1.2055124994,0.4637297335\C,-0.5951521695,0.9528487
231,0.040269213\C,-3.3007043679,0.0181156037,0.4425360205\C,-1.6338228
234,1.8162415972,0.1797139329\C,-2.9782168481,1.3699800303,0.461781159
8\C,3.8205342438,0.447724362,-0.4093407014\C,5.2368848113,0.7505234813
, -0.84821902\C,-0.2479137221,3.6863618196,-0.2317158413\H,1.6412409816
, -2.4105509004,-1.2363630566\H,1.4645059532,-0.667498854,-1.4469986411
\H,-0.8456712605,-3.5158117098,-1.033024412\H,2.3296209266,-2.08268440
25,1.1050821133\H,1.8375817623,-0.3962956162,1.0637249338\H,-3.1145087
998,-2.630528685,-0.4963924004\H,0.419064373,1.2606336324,-0.176265933
1\H,-4.3353145217,-0.3021273045,0.4851816498\H,-3.7370084805,2.1290161
373,0.5880625277\H,4.3233616223,-1.4885863903,0.0102323478\H,5.2159662
727,1.0629552576,-1.8924903886\H,5.9147089101,-0.0963882739,-0.7375803
998\H,5.6067622109,1.5884083025,-0.2571454866\H,-0.3650489187,4.765412
8849,-0.2827206971\H,0.4441896018,3.4185410758,0.5696032477\H,0.137349
7517,3.3068581404,-1.1808030453\O,-0.4258182162,-0.4965033326,1.831395
1653\O,-0.5467769454,-1.8282840348,2.3404161755\C,-1.549019451,-1.7763
864703,3.354236312\H,-2.5190554767,-1.5397910629,2.9102951123\H,-1.279
3477519,-0.9928482695,4.0682660205\C,-1.5622863831,-3.1222537422,4.011
0635944\H,-0.6214762246,-3.4552921592,4.4386221299\C,-2.6516968649,-3.
8820949541,4.0974853597\H,-3.5941636332,-3.5634243282,3.6650444065\H,-
2.6378984308,-4.838481406,4.605646796\

Zero-point correction= 0.360063 (Hartree/Particle)
Thermal correction to Energy= 0.382687
Thermal correction to Enthalpy= 0.383632
Thermal correction to Gibbs Free Energy= 0.305915
Sum of electronic and zero-point Energies= -1032.096825
Sum of electronic and thermal Energies= -1032.074200
Sum of electronic and thermal Enthalpies= -1032.073256
Sum of electronic and thermal Free Energies= -1032.150973

Product (*OO-CH₂-CH=CH₂ addition to C9)

\O,1.5063329657
,2.7589941262,0.183308245\O,-2.6956805133,1.1088199582,-0.5463886572\N
,2.1051902808,-2.7011848729,-0.0627253882\N,-3.4715908522,-0.996933964
, -0.8486244122\C,-0.0136752085,-2.0403244386,0.2223087244\C,0.83158176
55,-0.9011369975,0.2063887454\C,-1.505591162,-1.9736614875,0.342784374
5\C,2.1388820736,-1.330054258,0.0300653106\C,0.806705272,-3.1374714951
,0.0512792782\C,-2.1418889454,-1.5661208827,-0.9994882521\C,0.49216257

97,0.5255114742,0.4479825727\C,3.2396560426,-0.4400548255,-0.071208712
6\C,1.668367397,1.4098186038,0.1418266363\C,2.9527653982,0.9316875652,
-0.0323242484\C,-3.6385007459,0.3233925764,-0.5841440614\C,-5.05807096
92,0.7845355216,-0.338931394\C,0.1872433568,3.2840979693,0.0111502688\
H,-1.9199546719,-2.9268889385,0.681056503\H,-1.7636274182,-1.216591878
,1.0875499999\H,0.5672678741,-4.187948145,0.0095572721\H,-2.2018520536
,-2.4219450345,-1.6731527613\H,-1.5253424679,-0.8074325498,-1.47926170
7\H,2.9046919138,-3.2939847041,-0.2008561835\H,-0.4081104285,0.8263134
33,-0.0960120804\H,4.2518194163,-0.7929380772,-0.212553115\H,3.7442325
359,1.6598283677,-0.1615767605\H,-4.2702053615,-1.6065312257,-0.797788
9568\H,-5.8016316291,0.0069795724,-0.5159428959\H,-5.2606393223,1.6359
171214,-0.9879296009\H,-5.1341741142,1.1262572549,0.6941420067\H,0.303
5458498,4.3644789358,0.0334619138\H,-0.2274598788,2.9770986575,-0.9509
510202\H,-0.4727138544,2.9596672093,0.8151513658\O,0.038661273,0.74634
71363,1.821377918\O,1.0857106983,0.3239033291,2.6925421463\C,1.5474939
224,1.4871225907,3.3801472042\H,1.7380440373,2.2764054261,2.6485088312
\H,0.7898375163,1.8246458664,4.0932830506\C,2.8141343182,1.0882853257,
4.0723966598\H,3.5956913592,0.6947035229,3.4293510273\C,3.0054369683,1
.2118532939,5.3835029784\H,3.9463338091,0.9416152357,5.8468833221\H,2.
2240161129,1.5915163509,6.0330867024\
Zero-point correction= 0.360774 (Hartree/Particle)
Thermal correction to Energy= 0.383448
Thermal correction to Enthalpy= 0.384392
Thermal correction to Gibbs Free Energy= 0.305650
Sum of electronic and zero-point Energies= -1032.126124
Sum of electronic and thermal Energies= -1032.103450
Sum of electronic and thermal Enthalpies= -1032.102506
Sum of electronic and thermal Free Energies= -1032.181248

Product (*OO-CH₂-CH=CH₂ addition to C10)

\O,1.9639905517,-2.4051412089,-1.0
078021625\O,-2.8382145929,-1.275972641,-0.6606199589\N,1.8106398865,2.
7306181418,0.3788354534\N,-3.6885871818,0.4882382223,0.466158052\C,-0.
2265553569,1.900580541,-0.0845302294\C,0.7255622634,0.8118597273,-0.03
33502173\C,-1.689471917,1.7275584735,-0.3412340792\C,1.9829863051,1.37
96655705,0.2597346363\C,0.4765731476,3.0441638529,0.1718964094\C,-2.37
37814813,0.9967289566,0.826582509\C,0.5817372146,-0.5561360347,-0.2107
766358\C,3.1694546995,0.5907790151,0.358634001\C,1.7553690792,-1.45688
92066,0.0006938496\C,3.0637849369,-0.7470080426,0.2032690326\C,-3.8141
475687,-0.6393570597,-0.2771533415\C,-5.2245833773,-1.0771518818,-0.60
63554254\C,0.8021390255,-3.0966791988,-1.4697618335\H,-2.1724044143,2.
6934249495,-0.5106290043\H,-1.8296333995,1.1224799909,-1.2408433625\H,
0.1399365745,4.0676951776,0.2216585114\H,-2.4863959243,1.6644435841,1.
6810066103\H,-1.7619880151,0.1513960039,1.141357589\H,2.5393509679,3.3
979508826,0.5620537901\H,-0.3852482231,-1.0049914172,-0.3981213294\H,4
.1337556767,1.056955263,0.527738711\H,3.9293820451,-1.3964816787,0.236
1090608\H,-4.5140700123,0.9970203706,0.7316097301\H,-5.9898970122,-0.4
213876364,-0.1902022601\H,-5.3672990733,-2.0874722323,-0.2227854568\H,
-5.3305900676,-1.1142392421,-1.6906849207\H,1.1738295092,-3.9505155343
,-2.0313046789\H,0.1924190898,-3.44162393,-0.6345306394\H,0.2077088257
,-2.458817263,-2.1261694926\O,1.4958433561,-2.3133081325,1.1740078387\
O,1.1443813105,-1.453486538,2.2542917545\C,2.1237760872,-1.6522818989,
3.2715735724\H,3.1153651207,-1.5618651864,2.8207730497\H,2.0132427158,
-2.6478167169,3.7094438243\C,1.9007541794,-0.5747263246,4.2869645132\H
,1.9335736552,0.4425989982,3.9077074799\C,1.6901690484,-0.8144509478,5
.5790328131\H,1.6414000922,-1.8279465372,5.9624998227\H,1.563158053,-0
.008965581,6.2918156041\
Zero-point correction= 0.359997 (Hartree/Particle)
Thermal correction to Energy= 0.381899
Thermal correction to Enthalpy= 0.382843
Thermal correction to Gibbs Free Energy= 0.306242
Sum of electronic and zero-point Energies= -1032.115902

Sum of electronic and thermal Energies= -1032.094000
Sum of electronic and thermal Enthalpies= -1032.093056
Sum of electronic and thermal Free Energies= -1032.169657

Product (*OO-CH₂-CH=CH₂ addition to C11)

\O,0.7782549423

,-2.5624298555,-1.8009558105\O,-3.3156226954,-0.878494924,-0.098728268
\N,1.6356855752,2.8334581751,-1.1401572613\N,-3.481539905,0.9363637537
,1.2391022764\C,-0.4588171071,2.134159688,-0.6932610543\C,0.3189623802
,1.0082850709,-1.0596838355\C,-1.9061276082,2.0789422661,-0.3118251048
\C,1.6411528359,1.4593302512,-1.3345138536\C,0.3777997122,3.2336711795
,-0.7526761096\C,-2.0989208844,1.3330631672,1.0183062974\C,-0.03309361
65,-0.3692312355,-1.2360070964\C,2.6464251142,0.6186754244,-1.73975994
55\C,0.9451731637,-1.2394645775,-1.5832430506\C,2.3971921793,-0.852337
8333,-1.7144735665\C,-3.9944243961,-0.1608285927,0.6294985806\C,-5.453
5845017,-0.4594841771,0.8959351416\C,-0.5238314895,-3.0845906696,-1.57
25810308\H,-2.3303555979,3.0841008799,-0.2420271138\H,-2.4641084074,1.
5381109909,-1.0811708757\H,0.1636031533,4.2717257583,-0.552352655\H,-1.
.7787366015,1.9533809478,1.8559127802\H,-1.4917810106,0.4281760317,1.0
203885444\H,2.4232294561,3.4408693715,-1.2768213776\H,-1.0603342482,-0.
.6807482217,-1.0944587659\H,3.6434682248,0.9632156645,-1.9819573397\H,
2.8199536012,-1.3552863792,-2.5895079382\H,-4.0878818336,1.5193398362,
1.7899226451\H,-5.9150557325,0.2313906121,1.6021177157\H,-5.5308020171
,-1.4760149691,1.281399012\H,-5.9922999585,-0.4206766637,-0.0512819123
\H,-0.4528719545,-4.1531077972,-1.7558052125\H,-0.8359529512,-2.895544
032,-0.5433336726\H,-1.2460765702,-2.6329198328,-2.256893467\O,3.16434
75828,-1.5034762128,-0.6560192601\O,2.6185323954,-1.0679752976,0.58692
47107\C,3.6342243974,-0.3154735082,1.2443413951\H,3.8506010441,0.59367
31104,0.6779586545\H,4.5377041165,-0.9292042326,1.3088836896\C,3.09986
06958,0.0117627329,2.6053224922\H,2.8588822521,-0.8326461417,3.2433265
275\C,2.9207261497,1.259233173,3.0332853991\H,2.5502151946,1.470274046
4,4.029017456\H,3.1399779501,2.1081864519,2.3942918498\

Zero-point correction= 0.360300 (Hartree/Particle)

Thermal correction to Energy= 0.382126

Thermal correction to Enthalpy= 0.383070

Thermal correction to Gibbs Free Energy= 0.306727

Sum of electronic and zero-point Energies= -1032.121098

Sum of electronic and thermal Energies= -1032.099273

Sum of electronic and thermal Enthalpies= -1032.098329

Sum of electronic and thermal Free Energies= -1032.174672

Product (*OO-CH₂-CH=CH₂ addition to C12)

\O,-1.345105091

3,2.9237211602,0.1592794485\O,2.8999187084,1.0171685429,0.2942886553\N
,-2.12322584,-2.42466598,-0.8716066267\N,3.4231388328,-1.1332636087,0.
7560676893\C,0.0282265849,-1.8208702823,-0.7512499598\C,-0.8016271135,
-0.6644709479,-0.5553259147\C,1.5248631297,-1.8031369385,-0.7118180425
\C,-2.1184343405,-1.0843642218,-0.6393184688\C,-0.8235390647,-2.883307
0096,-0.9299471049\C,2.0346945237,-1.5674227466,0.7199163964\C,-0.4756
979759,0.6939436753,-0.2825093559\C,-3.2993586564,-0.2064739416,-0.447
7623197\C,-1.5516168554,1.5959965107,-0.1058778299\C,-2.8659085409,1.2
025292639,-0.2000093425\C,3.7509811378,0.1596586537,0.5148254648\C,5.2
252659245,0.4971210868,0.5356350154\C,-0.0038044393,3.3903713837,0.186
0105345\H,1.9376463871,-2.7350391583,-1.1065527036\H,1.8962213769,-0.9
870245666,-1.3375731576\H,-0.6107035311,-3.9256315581,-1.1053237092\H,
1.939670882,-2.4758040522,1.3151685906\H,1.4370097069,-0.791039355,1.1
964541544\H,-2.9480218832,-3.0007858285,-0.8719713803\H,0.5570099517,1.
.0024412557,-0.2049021779\H,-3.9854979383,-0.2540985463,-1.3038582785\
H,-3.6382330206,1.9531866675,-0.0930582249\H,4.1564425872,-1.808898162
7,0.8858994684\H,5.8599847893,-0.353167137,0.7864375523\H,5.3848813275
,1.2941382815,1.2617931324\H,5.5055354222,0.8797531431,-0.4461772416\H
,-0.0692845821,4.4560103513,0.3902615198\H,0.5749090316,2.8989224702,0

.9712582241\H,0.4885417993,3.2290623694,-0.7761019626\O,-4.1773916432,
-0.7307318925,0.5889885375\O,-3.40312552,-0.8671228486,1.7786295471\C,
-3.9204319542,0.0699261664,2.7238480624\H,-3.9427229972,1.0582857675,2
.2586388463\H,-4.9315024101,-0.2210495475,3.0201809963\C,-2.9786555524
,0.0532536702,3.8879901617\H,-1.9435875299,0.2894639789,3.6607711654\C
, -3.3619068983,-0.2099103146,5.1347683258\H,-4.3922462854,-0.457383377
2,5.3666487987\H,-2.6618401693,-0.1824394369,5.9605895044\\
Zero-point correction= 0.360587 (Hartree/Particle)
Thermal correction to Energy= 0.383258
Thermal correction to Enthalpy= 0.384202
Thermal correction to Gibbs Free Energy= 0.304501
Sum of electronic and zero-point Energies= -1032.122839
Sum of electronic and thermal Energies= -1032.100167
Sum of electronic and thermal Enthalpies= -1032.099223
Sum of electronic and thermal Free Energies= -1032.178924

Product (*OCCl₃ addition to C5)

\O,-0.889084
0999,3.4692648637,0.3765700441\O,2.8127331559,1.0706143163,-0.23911568
62\N,-2.7150529228,-1.5668049182,-0.9154926824\N,3.2346653441,-1.13867
65825,-0.0106554314\C,-0.5714821868,-1.5634339929,0.0238916674\C,-1.13
96689901,-0.1637543028,-0.0575703388\C,0.8764085029,-1.7431451379,-0.4
569649263\C,-2.4217529961,-0.2354497887,-0.5998795508\C,-1.5925577571,
-2.3405782665,-0.7256661259\C,1.9453559859,-1.4156665718,0.6015147206\
C,-0.572746279,1.0581049983,0.2899798981\C,-3.191907195,0.9092795707,-
0.7816316101\C,-1.334208244,2.2121963544,0.0959775624\C,-2.6344510895,
2.1296529824,-0.4235590064\C,3.5649737042,0.1155953037,-0.4072242225\C
,4.916226944,0.278634242,-1.0663475164\C,0.4428620988,3.5931359352,0.8
57655876\H,1.0099852815,-2.7712984271,-0.8038226883\H,1.0107883238,-1.
0795634022,-1.3126699732\H,-1.6188093308,-3.4123599088,-0.8275992716\H
,2.0628526937,-2.2428819641,1.299568231\H,1.6684801461,-0.5376657239,1
.1789406273\H,-3.4725076863,-1.8328563289,-1.52090476\H,0.4429622012,1
.1120056993,0.6534644264\H,-4.1914378847,0.8614871321,-1.1962083942\H,
-3.1878563835,3.0509278169,-0.5522063988\H,3.8721136543,-1.8951757425,
-0.1920310782\H,5.4927060527,-0.6459238547,-1.1059679606\H,5.478317989
6,1.0326990339,-0.515659826\H,4.7625039091,0.6513899817,-2.0794508985\
H,0.6132808609,4.6594607027,0.9798295614\H,0.5532600214,3.0915584624,1
.8231384914\H,1.159987607,3.1767120802,0.1473331357\O,-0.453320126,-2.
014535792,1.442184507\O,-1.7540506759,-1.9243736232,2.0209001679\C,-1.
8821437873,-2.9531394942,2.910966037\Cl,-1.7632452216,-4.5568812204,2.
1232159603\Cl,-0.6561196847,-2.858566103,4.2073193349\Cl,-3.5014855062
, -2.7393340097,3.5908411575\\
Zero-point correction= 0.296185 (Hartree/Particle)
Thermal correction to Energy= 0.320058
Thermal correction to Enthalpy= 0.321002
Thermal correction to Gibbs Free Energy= 0.238763
Sum of electronic and zero-point Energies= -2333.505756
Sum of electronic and thermal Energies= -2333.481883
Sum of electronic and thermal Enthalpies= -2333.480939
Sum of electronic and thermal Free Energies= -2333.563178

Product (*OCCl₃ addition to C6)

\O,0.5604368
206,3.521614902,0.6584723129\O,-3.1619541207,0.6827238237,0.199610094\
N,2.6911936907,-1.3687580511,-0.7673027664\N,-3.3037373617,-1.23923631
54,-0.9808206037\C,0.4149482978,-1.3373137303,-0.3456529036\C,0.918865
3281,-0.0449503594,-0.1661780795\C,-1.0029540662,-1.7575095913,-0.1794
468724\C,2.3246836435,-0.0844634673,-0.3671555082\C,1.5716874433,-2.25
28503944,-0.5985490652\C,-1.891276819,-1.2259558027,-1.3231728099\C,0.
2689905558,1.1624623007,0.1804144761\C,3.0970931516,1.0557156397,-0.21
04639755\C,1.0522093258,2.2934491093,0.3285602526\C,2.4520288521,2.240
2483793,0.1418621504\C,-3.8353722572,-0.2592441707,-0.2076836388\C,-5.

3051073866,-0.3835665368,0.1247564643\C,-0.8449602779,3.6193826248,0.8
352605972\H,-1.0821883264,-2.8454967876,-0.1112495457\H,-1.3888249404,
-1.3400070632,0.756466589\H,-1.7499340737,-1.8163991202,-2.2287968327\
H,-1.6168004964,-0.1949478175,-1.5441685684\H,3.6098128885,-1.72598257
86,-0.5568510855\H,-0.8034396312,1.1715331456,0.3254432891\H,4.1695937
275,1.0378062462,-0.3584724826\H,3.0121219051,3.1559700301,0.276478070
9\H,-3.8801646951,-2.0157287019,-1.2563728882\H,-5.7824727725,-1.24694
18928,-0.3391431203\H,-5.8084657056,0.5267727327,-0.2006374563\H,-5.40
87598169,-0.4524725265,1.2079926658\H,-1.0420325989,4.6612908602,1.073
0906458\H,-1.3745743705,3.3375675287,-0.0778595211\H,-1.1811634297,2.9
803898006,1.6551849296\H,1.4480494017,-2.9511033495,-1.4322464003\O,1.
7640024357,-3.2391235781,0.4662700243\O,1.7885126079,-2.5160222719,1.7
017884398\C,2.7465267208,-3.0707499123,2.5082918185\Cl,2.6292746603,-2
.1378019173,4.0041606643\Cl,2.4336674409,-4.7963804381,2.8242900006\Cl
,4.3934360091,-2.9017004988,1.819318789\

Zero-point correction= 0.297447 (Hartree/Particle)
Thermal correction to Energy= 0.320749
Thermal correction to Enthalpy= 0.321693
Thermal correction to Gibbs Free Energy= 0.240935
Sum of electronic and zero-point Energies= -2333.523298
Sum of electronic and thermal Energies= -2333.499996
Sum of electronic and thermal Enthalpies= -2333.499052
Sum of electronic and thermal Free Energies= -2333.579809

Product (*OCCl₃ addition to C7)

\O,-1.21396922,3.0921870191,-0.
1434016464\O,2.9571917388,1.0347427349,-0.0903378093\N,-2.3245372841,-
2.2175145189,-0.7549310493\N,3.4839290524,-1.1066921149,0.4052104884\C
,-0.0942105673,-1.716525566,-0.626435742\C,-0.8282722555,-0.5338137775
,-0.2884593546\C,1.3934516671,-1.7529650216,-0.7801436226\C,-2.2462621
346,-0.9438034602,-0.0979273905\C,-1.0143980576,-2.6943216342,-0.86741
91968\C,2.0930162275,-1.5021067455,0.5661477636\C,-0.4399992395,0.7963
062053,-0.2278293451\C,-3.2336479375,0.1140556898,-0.3857332456\C,-1.4
42872424,1.7635320622,-0.2109543301\C,-2.8290032004,1.4049870269,-0.36
09746536\C,3.8100213267,0.1653628394,0.0705302643\C,5.2833448467,0.464
8335287,-0.0925972585\C,0.1397399066,3.5137178603,0.0007130852\H,1.719
2870872,-2.7060853587,-1.2034548064\H,1.702354241,-0.9613665457,-1.469
6444512\H,-0.8423963295,-3.7081297648,-1.1977786606\H,2.057962555,-2.3
95482448,1.1894121508\H,1.5813143753,-0.7023321656,1.1008833718\H,-3.0
491970799,-2.848440436,-0.4424410578\H,0.6104682388,1.0559875805,-0.27
13622563\H,-4.2723979922,-0.1584984147,-0.5171944525\H,-3.5346342482,2
.2179272592,-0.4792656135\H,4.2135150895,-1.7928938643,0.4950175551\H,
5.4544754801,0.8103457406,-1.1123863676\H,5.9244194077,-0.3932184511,0
.1106332861\H,5.5444613714,1.2791540275,0.5832289607\H,0.1016907706,4.
5945884842,0.0998579756\H,0.5869958183,3.0671448966,0.8903437234\H,0.7
265232509,3.2380895878,-0.8771672545\O,-2.4266594323,-1.4069984846,1.3
676685498\O,-2.1502917322,-0.2896564152,2.2099973983\C,-3.0381600145,-
0.2970274709,3.2463244468\Cl,-4.7369780063,-0.1481726282,2.7085415886\
Cl,-2.88315479,-1.77902893,4.2368073533\Cl,-2.5858833159,1.1217120437,
4.2059076231\

Zero-point correction= 0.296653 (Hartree/Particle)
Thermal correction to Energy= 0.320109
Thermal correction to Enthalpy= 0.321053
Thermal correction to Gibbs Free Energy= 0.240420
Sum of electronic and zero-point Energies= -2333.495597
Sum of electronic and thermal Energies= -2333.472142
Sum of electronic and thermal Enthalpies= -2333.471197
Sum of electronic and thermal Free Energies= -2333.551830

Product (*OCCl₃ addition to C8)

\O,-1.555279
9515,3.1962194597,-0.088520702\O,2.8187606011,1.2743910885,-0.22900777

05\N,-2.4070581453,-2.1318240855,-0.6294362993\N,3.4290663938,-0.85574
02128,0.215070676\C,-0.205988713,-1.5486671697,-0.6052933754\C,-0.9860
479163,-0.4656037132,0.0911215447\C,1.2716267752,-1.4881110157,-0.8175
088207\C,-2.4032700293,-0.834246101,-0.1921513429\C,-1.0874092665,-2.4
977347058,-0.960176534\C,2.0614993547,-1.2760546964,0.4846552622\C,-0.
6669888423,0.9628274138,-0.1096773675\C,-3.4284095784,0.0948325259,-0.
0881665741\C,-1.6965780344,1.848237789,-0.0412920265\C,-3.0770007195,1
.4279186018,0.0439464043\C,3.7011089433,0.4251182182,-0.1331529829\C,5
.1521656554,0.7592380509,-0.3993238175\C,-0.2235791892,3.6931623218,-0
.1453154577\H,1.6182109518,-2.3932417478,-1.3235670453\H,1.4940493055,
-0.6393814933,-1.4722097631\H,-0.9067403475,-3.4491419161,-1.437945920
6\H,2.0864308002,-2.190055752,1.0777159076\H,1.5891495838,-0.503299719
7,1.0876357469\H,-3.2109334782,-2.5606180826,-1.0562191621\H,0.3732816
441,1.25012742,-0.1828741932\H,-4.468088846,-0.1999391601,-0.162873572
4\H,-3.8252128779,2.2032163527,0.1281599938\H,4.1784965895,-1.52481803
31,0.255272104\H,5.2433776187,1.108879807,-1.4280412785\H,5.8254185542
,-0.0841559115,-0.243595192\H,5.4415684481,1.5789881466,0.258176468\H,
-0.3105007774,4.7759927521,-0.1406936037\H,0.3492465844,3.3546842711,0
.7205972488\H,0.2739521699,3.360186736,-1.0587970888\O,-0.7485541394,-
0.5754707592,1.6062553035\O,-0.8717895355,-1.962478064,1.987918318\C,-
1.4592043536,-2.0176430244,3.2157337893\Cl,-3.1055407542,-1.3281527202
,3.2268316041\Cl,-0.4790873554,-1.1933317162,4.4630896989\Cl,-1.537335
0929,-3.7597475246,3.5703730007\

Zero-point correction= 0.295904 (Hartree/Particle)
Thermal correction to Energy= 0.319621
Thermal correction to Enthalpy= 0.320565
Thermal correction to Gibbs Free Energy= 0.239568
Sum of electronic and zero-point Energies= -2333.486484
Sum of electronic and thermal Energies= -2333.462767
Sum of electronic and thermal Enthalpies= -2333.461823
Sum of electronic and thermal Free Energies= -2333.542820

Product (*OCCl₃ addition to C9)

\O,1.5828767845,2.7858884551,-0
.5462762535\O,-2.5938031905,1.1288589966,-0.4854868656\N,2.1842812125,
-2.6530593383,-0.1653133148\N,-3.4396061583,-0.9689757772,-0.541955241
5\C,0.1044204274,-1.9477622313,0.2660058638\C,0.9445172701,-0.82431204
97,0.0408983082\C,-1.3664925261,-1.854472883,0.5329748325\C,2.22711514
03,-1.2817463078,-0.2217863181\C,0.904295329,-3.0627459771,0.126842456
\C,-2.140588384,-1.5802392242,-0.7710282785\C,0.6446853879,0.618999633
6,0.1756401144\C,3.3117898217,-0.4147940543,-0.5237334746\C,1.76126778
71,1.4580807004,-0.3626148096\C,3.0276816899,0.9497237761,-0.608749288
\C,-3.5557084642,0.3723640101,-0.3787981088\C,-4.937732513,0.895921760
7,-0.0602163256\C,0.2682445313,3.3345074685,-0.4249643517\H,-1.7419562
442,-2.7635546006,1.008987152\H,-1.5483101865,-1.023040156,1.218658685
1\H,0.6632417815,-4.1096444614,0.2190865257\H,-2.2832986273,-2.5024882
747,-1.3352483058\H,-1.5706607335,-0.8930965998,-1.3949443407\H,2.9653
210638,-3.265237533,-0.3254024968\H,-0.3303937169,0.8847944099,-0.2406
030484\H,4.3076083789,-0.7893300965,-0.7150464218\H,3.7975157266,1.653
1701229,-0.8995603176\H,-4.2447462079,-1.5507475226,-0.3830869942\H,-5
.7088340581,0.1258001085,-0.0908668483\H,-5.1808264143,1.6821273435,-0
.7743784108\H,-4.9145688653,1.3435043975,0.9340472622\H,0.3895703072,4
.4012293067,-0.5917782132\H,-0.3993823581,2.9162626143,-1.1800094789\H
,-0.1391279271,3.1563959213,0.5695988755\O,0.3626819914,0.9720656059,1
.5932476466\O,1.4840581679,0.5175702882,2.3581596525\C,1.7382309154,1.
4409336654,3.3331055648\Cl,0.3421791847,1.6463131876,4.4317930571\Cl,3
.1079104886,0.7489737299,4.2211042743\Cl,2.1867012275,3.0317946549,2.6
646260662\

Zero-point correction= 0.297938 (Hartree/Particle)
Thermal correction to Energy= 0.321395
Thermal correction to Enthalpy= 0.322339
Thermal correction to Gibbs Free Energy= 0.241377

Sum of electronic and zero-point Energies= -2333.513061
Sum of electronic and thermal Energies= -2333.489605
Sum of electronic and thermal Enthalpies= -2333.488660
Sum of electronic and thermal Free Energies= -2333.569622

Product (*OCCl₃ addition to C10)

\O,2.0271551318,-2.34662697,-1.
0144246023\O,-2.6699880055,-1.3029127442,-0.4456392239\N,1.8457540678,
2.8979707648,-0.0521635299\N,-3.5568406233,0.5128292988,0.5640551707\C
, -0.1975163967,1.9964835291,-0.3123960977\C,0.7840278307,0.9348166858,
-0.2490218367\C,-1.6687574657,1.771179952,-0.4561725722\C,2.0446168685
,1.5481332374,-0.0842092898\C,0.4924924937,3.1686158026,-0.1857845899\
C,-2.2540895258,1.1132387652,0.8058851739\C,0.662481308,-0.4440340994,
-0.3188979927\C,3.2531184582,0.7920834365,-0.0058629925\C,1.869986419,
-1.2921628062,-0.1218848756\C,3.1703924893,-0.5547479438,-0.0526735663
\C,-3.6592845081,-0.6839191656,-0.0653427901\C,-5.0575934604,-1.222417
0834,-0.2707562753\C,0.8428506609,-3.070990179,-1.3622718944\H,-2.1885
400469,2.7098209646,-0.6636779451\H,-1.8495352627,1.0977534688,-1.2980
977834\H,0.1348294281,4.1861096503,-0.183381789\H,-2.3561323826,1.8460
242499,1.6064201953\H,-1.5844855861,0.3274923244,1.155750409\H,2.56561
64713,3.5909324547,0.0570789948\H,-0.3026529158,-0.9252990047,-0.41154
41297\H,4.214310427,1.2860360671,0.0751315842\H,4.0477200194,-1.185915
9853,-0.0086529518\H,-4.3934273699,0.9999986833,0.8354750797\H,-5.8357
640351,-0.5656311845,0.1188841862\H,-5.1257108077,-2.1932912746,0.2202
635176\H,-5.2150815001,-1.3771412297,-1.3382369712\H,1.1913123364,-3.9
764683928,-1.8521363149\H,0.2657257923,-3.3293790771,-0.4744171482\H,0
.2275865581,-2.4923716675,-2.052535252\O,1.7046660551,-2.0643337083,1.
1665928378\O,1.3943852736,-1.1008518421,2.1745450555\C,1.9663663674,-1
.5128442534,3.3447564615\Cl,3.7471391906,-1.6038451259,3.2468330198\Cl
,1.3363614662,-3.099075331,3.8687531539\Cl,1.491729609,-0.2594437367,4
.5073991047\

Zero-point correction= 0.296951 (Hartree/Particle)
Thermal correction to Energy= 0.320495
Thermal correction to Enthalpy= 0.321439
Thermal correction to Gibbs Free Energy= 0.240108
Sum of electronic and zero-point Energies= -2333.503342
Sum of electronic and thermal Energies= -2333.479798
Sum of electronic and thermal Enthalpies= -2333.478854
Sum of electronic and thermal Free Energies= -2333.560185

Product (*OCCl₃ addition to C11)

\O,1.5963900
43,-2.6802732313,-0.7647013332\O,-2.8298877243,-1.3128093752,-0.231380
214\N,1.8579282598,2.7921112688,-0.258809243\N,-3.5399427694,0.5534099
346,0.8283006401\C,-0.2253735716,1.9375875485,-0.3443395158\C,0.700057
1595,0.8689275411,-0.4206112197\C,-1.7143784059,1.7724053736,-0.349148
7461\C,2.0123825571,1.4180537702,-0.355725859\C,0.5189423058,3.0991227
777,-0.2404340499\C,-2.1963365675,1.0989742289,0.9467424298\C,0.506426
3273,-0.5400367577,-0.5863795282\C,3.1475393337,0.6507988148,-0.414695
0987\C,1.600515157,-1.3387706934,-0.6061761524\C,2.9996282737,-0.82788
04758,-0.3845678368\C,-3.7517754963,-0.6415448098,0.2234493213\C,-5.18
68503343,-1.1120665439,0.1427214956\C,0.3210684876,-3.3046074214,-0.85
20406062\H,-2.2143797295,2.7353369975,-0.4801427301\H,-2.0066924692,1.
1326003333,-1.1861652365\H,0.1867337402,4.1221605429,-0.1607339199\H,-
2.1830512286,1.8076285116,1.7751987636\H,-1.5283727019,0.2756206708,1.
1991557998\H,2.6080920122,3.4525973951,-0.1619526927\H,-0.4968355054,-
0.9326245977,-0.6931466846\H,4.1458237578,1.0643308519,-0.3794825648\H
,3.6844225546,-1.3348772072,-1.0710899979\H,-4.3287450134,1.0865943623
,1.151661815\H,-5.8928892489,-0.4296167368,0.6165776828\H,-5.253877035
1,-2.0896452934,0.6202083881\H,-5.4520532373,-1.2353093507,-0.90754696
09\H,0.5165548392,-4.3697780315,-0.9363151068\H,-0.2684617555,-3.09540
81901,0.0428218597\H,-0.2208575916,-2.9499999227,-1.7317515263\O,3.515

6180341,-1.3962495314,0.8768003835\O,2.6352296297,-0.9267729103,1.9042
055516\C,3.3701367794,-0.7115328262,3.0331190619\Cl,2.16383605,-0.1879
511214,4.2230766239\Cl,4.1801760546,-2.199224545,3.5921154713\Cl,4.603
9095394,0.5684720894,2.8201585056\

Zero-point correction= 0.297402 (Hartree/Particle)
Thermal correction to Energy= 0.320931
Thermal correction to Enthalpy= 0.321875
Thermal correction to Gibbs Free Energy= 0.239846
Sum of electronic and zero-point Energies= -2333.509069
Sum of electronic and thermal Energies= -2333.485540
Sum of electronic and thermal Enthalpies= -2333.484596
Sum of electronic and thermal Free Energies= -2333.566625

Product (*OH addition to C12)

\O,0.4132869294,2.9099234009,-1.3794435198\O,4.2898471179,1
.1482809461,0.4499690306\N,-0.2266436783,-2.5507401664,-1.5685672758\N
,4.549670719,-0.8413038179,1.4892367479\C,1.7954812009,-1.8887234754,-
0.8722102504\C,0.9948426853,-0.7336547502,-1.1701533625\C,3.1992810668
, -1.8317321268,-0.3544638122\C,-0.2412270357,-1.1893876419,-1.59696814
6\C,1.0037882246,-2.9831226911,-1.1207620523\C,3.2312028277,-1.3117423
831,1.0931515611\C,1.2745760403,0.6575731794,-1.0730623337\C,-1.377733
8614,-0.3094984471,-1.9500301252\C,0.2408056563,1.5559917167,-1.430712
4451\C,-0.9920089006,1.1254627532,-1.8626726774\C,4.9880598947,0.38413
21581,1.1112962667\C,6.3838257973,0.7673964981,1.5491448639\C,1.678821
2931,3.4002612026,-0.9576068088\H,3.6770724562,-2.8130363168,-0.410279
6268\H,3.7849702435,-1.1436772953,-0.9699146209\H,1.2194717857,-4.0351
845323,-1.0251054753\H,2.9182295499,-2.0913665319,1.7879475414\H,2.540
217398,-0.4752833542,1.1952598466\H,-1.02255144,-3.1393639551,-1.74856
34294\H,2.2403652411,0.9954529343,-0.7258049409\H,-1.8106323834,-0.551
3615103,-2.9292022176\H,-1.7345070044,1.862752504,-2.1346185881\H,5.16
92324924,-1.4506394922,1.9951888168\H,6.8688095082,0.0065369577,2.1612
138559\H,6.3236218974,1.6993409428,2.1110331042\H,6.9858649288,0.95321
41659,0.6592535054\H,1.5963706072,4.4835225144,-0.9887112502\H,1.91162
86472,3.0760487642,0.0588557906\H,2.4737026075,3.0716674094,-1.6311944
347\O,-2.5589108523,-0.6394094042,-1.1303705294\O,-2.1621564297,-0.451
5302697,0.2319947304\C,-3.2318231859,0.0561723213,0.9197918365\Cl,-4.6
143786735,-1.0772752044,0.9035636527\Cl,-2.6171935227,0.236571067,2.57
18595108\Cl,-3.7643867543,1.6350247092,0.2921485971\

Zero-point correction= 0.297069 (Hartree/Particle)
Thermal correction to Energy= 0.320687
Thermal correction to Enthalpy= 0.321631
Thermal correction to Gibbs Free Energy= 0.238522
Sum of electronic and zero-point Energies= -2333.509029
Sum of electronic and thermal Energies= -2333.485411
Sum of electronic and thermal Enthalpies= -2333.484467
Sum of electronic and thermal Free Energies= -2333.567575

TS-C1 (*OH)

\O,-1.7480701461,3.012245015
4,0.142970656\O,2.7021517306,1.1507489723,-0.0916722792\N,-2.470201329
8,-2.424614389,-0.106981049\N,3.2393729078,-0.94109118,0.5827588998\C,
-0.3330688879,-1.7692036061,-0.3486060874\C,-1.1566444022,-0.604274179
2,-0.1632429778\C,1.153283432,-1.7381924077,-0.5211029805\C,-2.4835770
678,-1.0480912984,-0.0154703393\C,-1.1762414885,-2.8489223117,-0.30697
07258\C,1.849518423,-1.3294905496,0.7863694484\C,-0.8518165823,0.77048
02646,-0.1199444376\C,-3.5369599865,-0.1460093357,0.1800575758\C,-1.89
78241836,1.6558490624,0.0752514413\C,-3.2287347018,1.1988133312,0.2243
588192\C,3.5559539158,0.2883843086,0.1248803838\C,5.0150924706,0.56254
48667,-0.1152602524\C,-0.428421531,3.5174357488,0.0302504218\H,1.52808
44978,-2.7094735608,-0.8547869285\H,1.4163554564,-1.0019135663,-1.2863
274522\H,-0.9526620289,-3.8993698214,-0.4130072838\H,1.8242865639,-2.1
469870994,1.5069242033\H,1.3341151051,-0.4762597128,1.2256937432\H,-3.

2755441003,-3.0218342303,-0.0514805066\H,0.1723220081,1.1009031449,-0.2359028559\H,-4.560839143,-0.481411459,0.2943388283\H,-4.0006743423,1.9423663772,0.3749879178\H,3.9709991104,-1.62294838,0.6936943554\H,5.7153216503,-0.0683394528,0.4284914295\H,5.1892246,1.7136101333,0.2916469837\H,5.2442562355,0.6311678549,-1.1766169035\H,-0.5128599198,4.5967659781,0.126287217\H,0.2106708288,3.1221737812,0.8242260489\H,0.0057201953,3.2646515819,-0.940553566\O,4.8756259499,2.9348128522,0.5123302696\H,3.9258783004,2.8467162968,0.2864079724\

Zero-point correction= 0.286879 (Hartree/Particle)
Thermal correction to Energy= 0.304622
Thermal correction to Enthalpy= 0.305566
Thermal correction to Gibbs Free Energy= 0.239136
Sum of electronic and zero-point Energies= -840.342179
Sum of electronic and thermal Energies= -840.324437
Sum of electronic and thermal Enthalpies= -840.323492
Sum of electronic and thermal Free Energies= -840.389922

TS-C1b (*OH)

\O,-1.7952249045,2.972020853
5,0.0488274288\O,2.6364050446,1.229271051,-0.1675094734\N,-2.4282635869,-2.4818689629,-0.0290465979\N,3.2523455823,-0.8439573067,0.5315642455\C,-0.3055836684,-1.7965955079,-0.317393967\C,-1.1482795729,-0.6416348735,-0.1574615597\C,1.1776698287,-1.7413729673,-0.5092870728\C,-2.4656744175,-1.1035564777,0.0196827047\C,-1.1284638427,-2.8890495676,-0.2319052355\C,1.8849296745,-1.2779619043,0.7746512292\C,-0.8661654702,0.7385368697,-0.1595443742\C,-3.5319609534,-0.213558401,0.1993391309\C,-1.9247618015,1.6117131263,0.021548471\C,-3.2461901669,1.1372949492,0.1991641156\C,3.5048865091,0.3909887529,0.0641427685\C,4.9535482688,0.7456763349,-0.1792592844\C,-0.4874465152,3.4925693827,-0.1246946057\H,1.5694365149,-2.7134682491,-0.8196417125\H,1.4151506238,-1.0229522293,-1.2993987338\H,-0.886944789,-3.9381154254,-0.3070337816\H,1.905244289,-2.0806800858,1.5116553904\H,1.3419424581,-0.4374361322,1.2064931023\H,-3.2218738773,-3.0914153594,0.0540316152\H,0.1513476701,1.0825525896,-0.2943569835\H,-4.5487958313,-0.5621593063,0.3353197358\H,-4.0292800223,1.8718047312,0.3359825037\H,4.0315241089,-1.4749078406,0.6594791968\H,5.63947863,-0.1680500139,0.1710061631\H,5.2619209182,1.5975177378,0.4244109889\H,5.1438201063,0.9254188638,-1.2359348244\H,-0.5869865736,4.5733247308,-0.0647069028\H,0.1853350078,3.1360231027,0.6593974832\H,-0.0806630696,3.2107079153,-1.0993596948\O,6.1499835221,-1.4052382895,0.4571022002\H,6.6516771362,-1.567023691,-0.3623723698\

Zero-point correction= 0.286808 (Hartree/Particle)
Thermal correction to Energy= 0.304744
Thermal correction to Enthalpy= 0.305688
Thermal correction to Gibbs Free Energy= 0.238955
Sum of electronic and zero-point Energies= -840.343095
Sum of electronic and thermal Energies= -840.325159
Sum of electronic and thermal Enthalpies= -840.324215
Sum of electronic and thermal Free Energies= -840.390949

TS-C3 (*OH)

\O,-1.9089317796,2.919400017
7,0.0528842123\O,3.0241134978,1.3523830015,0.2327433445\N,-2.4288971775,-2.5443643057,0.1320758545\N,3.2665005142,-0.9022284271,0.2839161436\C,-0.3485445404,-1.8301592543,-0.3320593448\C,-1.1968459879,-0.6842016989,-0.135187748\C,1.1156104757,-1.7755347619,-0.634277706\C,-2.4875873422,-1.1659894947,0.1515972123\C,-1.1429205623,-2.9357221766,-0.1591223282\C,1.8834394982,-1.1593898564,0.5342164542\C,-0.9493034313,0.7025930586,-0.1875938749\C,-3.5568614856,-0.293989349,0.3950561233\C,-2.0083661833,1.558804615,0.0590402371\C,-3.3019396053,1.0607057792,0.3469132297\C,3.7514245886,0.3709600922,0.1739251257\C,5.2464439281,0.4932474168,-0.0130741287\C,-0.6285580332,3.4719164435,-0.2082907222\H,1.5031275821,-2.7740911074,-0.8527144808\H,1.2962864939,-1.1497333842,-1.51

6146064\H,-0.8853397897,-3.981329358,-0.2329843694\H,1.8034143765,-1.9
235993788,1.4294758299\H,1.4262022371,-0.240060676,0.8911411778\H,-3.2
043756199,-3.1643099547,0.2849979891\H,0.0434806109,1.0723980361,-0.40
75010889\H,-4.5518002196,-0.6612461632,0.6158862287\H,-4.0873503514,1.
7821995643,0.530380606\H,3.8988216292,-1.6796639532,0.1827353265\H,5.7
332792111,-0.4586784635,-0.2262068737\H,5.6715539561,0.9129709496,0.89
99791125\H,5.4375920373,1.1934452959,-0.8249105903\H,-0.7511772205,4.5
496472292,-0.1438692655\H,0.1033823268,3.1367371773,0.5307295378\H,-0.
2845640497,3.1995733694,-1.2096376095\O,1.3785368714,-2.9648763648,2.2
802707193\H,0.4247706446,-2.8877665679,2.0828088899\

Zero-point correction= 0.285853 (Hartree/Particle)
Thermal correction to Energy= 0.303508
Thermal correction to Enthalpy= 0.304452
Thermal correction to Gibbs Free Energy= 0.237495
Sum of electronic and zero-point Energies= -840.346586
Sum of electronic and thermal Energies= -840.328930
Sum of electronic and thermal Enthalpies= -840.327986
Sum of electronic and thermal Free Energies= -840.394944

TS-C4 (*OH)

\O,-1.7483965278,2.983583630
2,0.1645360324\O,2.5429809774,1.254990637,-0.1434491909\N,-2.505939384
6,-2.4388413151,-0.204499797\N,3.192876482,-0.789254073,0.5750459309\C
, -0.3471295125,-1.8146187477,-0.2545983633\C,-1.1656061046,-0.63560423
51,-0.1062275344\C,1.1255359754,-1.8452140395,-0.3477967825\C,-2.50536
36777,-1.0626176999,-0.0747152236\C,-1.2151046312,-2.8807134886,-0.320
3506489\C,1.8346201743,-1.2193880357,0.860019824\C,-0.8567382165,0.736
4888567,-0.0350102703\C,-3.5631837436,-0.1551188917,0.050029168\C,-1.9
077141181,1.6308067275,0.0853873442\C,-3.2495340295,1.1866671002,0.132
3973534\C,3.4350262953,0.4197079279,0.0176810747\C,4.8515334318,0.6809
701814,-0.429439147\C,-0.419974334,3.4796953167,0.105389279\H,1.501347
868,-2.8503058835,-0.5538519884\H,1.4516737451,-1.241976166,-1.3040086
75\H,-0.9981648292,-3.9306926197,-0.4409620372\H,1.8645256071,-1.94088
63613,1.6788256612\H,1.2868204725,-0.3471259364,1.2085693091\H,-3.3232
176376,-3.0229502591,-0.2173580952\H,0.1715997013,1.0688480556,-0.0803
968328\H,-4.5951915981,-0.4839274536,0.0757587142\H,-4.0248595094,1.93
57005771,0.2279185997\H,3.9302576547,-1.4746954727,0.5610756083\H,5.57
84991702,0.0295697616,0.0564532254\H,5.0953025499,1.7225909673,-0.2291
553337\H,4.8926935849,0.5178961948,-1.5087957819\H,-0.5037301745,4.560
7335867,0.1792581971\H,0.1802171374,3.0948666856,0.9334535928\H,0.0578
234389,3.2074579056,-0.8389605136\O,1.9679280345,-0.483622702,-2.42092
32768\H,1.8918105382,0.389913679,-1.9866969717\

Zero-point correction= 0.287006 (Hartree/Particle)
Thermal correction to Energy= 0.304757
Thermal correction to Enthalpy= 0.305701
Thermal correction to Gibbs Free Energy= 0.240385
Sum of electronic and zero-point Energies= -840.351620
Sum of electronic and thermal Energies= -840.333870
Sum of electronic and thermal Enthalpies= -840.332926
Sum of electronic and thermal Free Energies= -840.398241

TS-C13 (*OH)

\O,-1.7452703453,2.884090254
7,-0.1785228234\O,2.6198867376,0.7559826996,-0.4459829019\N,-2.7330070
881,-2.506611761,0.0958733473\N,3.0670869739,-1.2640494579,0.454885033
2\C,-0.5760658596,-1.9857178553,-0.2715823792\C,-1.3382639175,-0.76945
02204,-0.1772053907\C,0.9032636167,-2.0464126736,-0.4898255241\C,-2.67
98247328,-1.1299306416,0.0541168994\C,-1.4666583177,-3.0121475528,-0.0
987869122\C,1.6663410119,-1.542180187,0.7453332514\C,-0.9690999014,0.5
848974728,-0.272202184\C,-3.682213762,-0.1630439975,0.2015421078\C,-1.
9657928894,1.5312390576,-0.1232271801\C,-3.3093893662,1.1634019685,0.1
124517047\C,3.4401993355,-0.1129547218,-0.1408570654\C,4.9133627819,0.

0718201835,-0.4161973544\C,-0.4735683771,3.3278841677,-0.5215432779\H,
1.2195343078,-3.0646579193,-0.7312124769\H,1.174475262,-1.4080153692,-
1.3353530769\H,-1.2960354859,-4.0776200138,-0.1066549709\H,1.623035341
9,-2.2776894732,1.5487776719\H,1.2141748605,-0.6204358026,1.1109072556
\H,-3.5616639641,-3.0550734726,0.23982469\H,0.0656039469,0.8544426458,
-0.4358410628\H,-4.7151621753,-0.4351894506,0.3815479713\H,-4.03771324
7,1.9561139313,0.2226399747\H,3.7667369123,-1.9576691429,0.6579241647\
H,5.5205774534,-0.7787465963,-0.1064311533\H,5.2498865339,0.966707506,
0.1079562188\H,5.0449420142,0.2430429058,-1.4846436717\H,-0.5084264945
,4.4108054953,-0.5958400183\H,0.3063669011,3.0944753847,0.3487476798\H
,-0.0902912481,2.8578163599,-1.4299874363\O,1.3817552468,2.8222683435,
1.1830402862\H,1.8501419339,2.1725289324,0.6177336036\
Zero-point correction= 0.286894 (Hartree/Particle)
Thermal correction to Energy= 0.304655
Thermal correction to Enthalpy= 0.305599
Thermal correction to Gibbs Free Energy= 0.239477
Sum of electronic and zero-point Energies= -840.351444
Sum of electronic and thermal Energies= -840.333683
Sum of electronic and thermal Enthalpies= -840.332739
Sum of electronic and thermal Free Energies= -840.398861

TS-N1 (*OH)

\O,-1.8134724843,2.966847196
9,-0.092523986\O,2.6342411015,1.2105880356,0.0679096234\N,-2.345396628
5,-2.4965943933,-0.0013158401\N,3.2516841743,-0.7625832456,1.006902747
1\C,-0.2193497862,-1.7820371409,-0.1373158887\C,-1.0887474367,-0.63734
05663,-0.0948114013\C,1.2726126402,-1.7177163495,-0.2103925979\C,-2.40
84068273,-1.117981871,-0.0107088633\C,-1.0291075092,-2.886894898,-0.07
7337757\C,1.8738617927,-1.2006971573,1.1138925108\C,-0.8315343087,0.74
73587949,-0.1286649099\C,-3.5011328284,-0.2437384434,0.0426791648\C,-1
.9165669779,1.6054790685,-0.0731699878\C,-3.2397775622,1.1114933834,0.
0116375932\C,3.5194131381,0.3977570659,0.2883124678\C,4.9517514565,0.6
007809303,-0.1259948056\C,-0.5061784362,3.5091265722,-0.1794401481\H,1
.6805976434,-2.7071468906,-0.4367692517\H,1.5742520452,-1.0388726468,
-1.0132569408\H,-0.7650814993,-3.9331997135,-0.0893053297\H,1.819671311
2,-1.9683067716,1.8851850441\H,1.2968073193,-0.3357128812,1.4469853838
\H,-3.1334780252,-3.1175350555,0.0421631858\H,0.186197181,1.1083419471
, -0.1951538523\H,-4.5195527708,-0.6077261806,0.1058455698\H,-4.0443024
592,1.8342525441,0.0510127769\H,4.0435355182,-1.5935085366,0.912295663
2\H,5.6375993507,0.2650271472,0.6514477169\H,5.1023428684,1.6549535709
, -0.3464126977\H,5.1532292419,0.0044977016,-1.0176245647\H,-0.63076399
91,4.5887546989,-0.1750411112\H,0.1035014034,3.2018856279,0.6740810539
\H,-0.0139346888,3.1963127279,-1.1038757187\O,4.6405935535,-2.42379813
27,0.1670407077\H,3.9637340385,-2.9195942986,-0.322476837\
Zero-point correction= 0.286295 (Hartree/Particle)
Thermal correction to Energy= 0.304469
Thermal correction to Enthalpy= 0.305413
Thermal correction to Gibbs Free Energy= 0.238586
Sum of electronic and zero-point Energies= -840.340103
Sum of electronic and thermal Energies= -840.321929
Sum of electronic and thermal Enthalpies= -840.320985
Sum of electronic and thermal Free Energies= -840.387812

TS-N2 (*OH)

\O,-1.776
5176369,2.9424654985,0.0425705015\O,2.4761781246,1.0993030675,-0.01409
14394\N,-2.5725185747,-2.4431053961,-0.6270552565\N,3.090392764,-0.998
5899208,0.558293048\C,-0.3979503845,-1.8283511982,-0.605070879\C,-1.22
01914379,-0.6435234458,-0.4140588428\C,1.0927075963,-1.8053635633,-0.6
89696859\C,-2.5574530185,-1.076181347,-0.3989186735\C,-1.2636898756,-2
.883429306,-0.6852146148\C,1.7155867193,-1.4561215056,0.6755214337\C,-
0.8973019384,0.70732568,-0.2893846296\C,-3.6108965922,-0.1753109471,-0

.230171975\C,-1.9536648137,1.6049006806,-0.110072037\C,-3.2924188938,1
.1646712859,-0.0772963192\C,3.3656454111,0.2792962266,0.1977652851\C,4
.8268146127,0.6466754829,0.0727061758\C,-0.4406803549,3.43060987,0.023
9155177\H,1.4794358476,-2.7632387948,-1.0444433373\H,1.4010730769,-1.0
352308528,-1.4025163882\H,-1.0575668471,-3.9349355818,-0.8100381798\H,
1.6932964377,-2.3217421091,1.3373601329\H,1.1438963759,-0.6570540128,1
.1461460911\H,-3.3698727917,-3.074207595,-0.2887958706\H,0.135665852,1
.0294538561,-0.3251187241\H,-4.6409908267,-0.5090099825,-0.2150178582\
H,-4.0646134896,1.9091448447,0.0645141942\H,3.8475512976,-1.649026872,
0.6813623823\H,5.5015517644,-0.1690480542,0.3329683826\H,5.022892822,1
.4996701872,0.722146576\H,5.0173445211,0.9592208552,-0.9543294336\H,-0
.5181836651,4.503495303,0.1756089973\H,0.1517784027,2.9809577059,0.823
3047216\H,0.0357687766,3.2239889884,-0.9367690583\O,-3.9248400867,-3.7
57636715,0.8660301437\H,-3.7813285745,-3.2052177826,1.6524860824\
Zero-point correction= 0.287092 (Hartree/Particle)
Thermal correction to Energy= 0.305743
Thermal correction to Enthalpy= 0.306687
Thermal correction to Gibbs Free Energy= 0.238030
Sum of electronic and zero-point Energies= -840.348411
Sum of electronic and thermal Energies= -840.329760
Sum of electronic and thermal Enthalpies= -840.328816
Sum of electronic and thermal Free Energies= -840.397473

TS-C5 (*OH)

\O,-1.3852407946,3.224634333
5,0.2370561224\O,2.5704773951,1.138699247,-0.2844006298\N,-2.712269957
3,-2.0479721788,-0.5439320756\N,3.1852785677,-0.9700532399,0.253729209
8\C,-0.4982431265,-1.6883887819,-0.2326185562\C,-1.2060672669,-0.41863
99493,-0.1382947974\C,0.9747977685,-1.8077085156,-0.4949086672\C,-2.57
53942994,-0.6848002942,-0.2876047816\C,-1.4852152779,-2.6312147323,-0.
5577827501\C,1.8502128097,-1.3623884536,0.6894421218\C,-0.7469915456,0
.8940870897,0.0328851628\C,-3.5295457036,0.3310637031,-0.2246538593\C,
-1.6965007769,1.9072987463,0.0839335267\C,-3.0737917302,1.6239620676,-
0.0294771028\C,3.4413307683,0.2735363985,-0.2112582857\C,4.8637019518,
0.5549191414,-0.6435886392\C,-0.005402222,3.5482634201,0.3498557188\H,
1.2190373697,-2.838169897,-0.764347413\H,1.2170862943,-1.1744871294,-1
.3541464736\H,-1.3653815395,-3.6900709789,-0.7153891903\H,1.9380635742
,-2.1626602172,1.4174912867\H,1.400668154,-0.5129221258,1.1976772448\H
,-3.5846050435,-2.53778149,-0.6384987964\H,0.3144929004,1.0956479796,0
.0879011398\H,-4.5880654352,0.129574081,-0.3351971287\H,-3.7658923941,
2.4542185382,0.0234719908\H,3.9326615879,-1.642333736,0.2834448079\H,5
.542785146,-0.2798658428,-0.4680620856\H,5.2200326934,1.4317155887,-0.
1031620557\H,4.8590322776,0.7981268343,-1.7066272174\H,0.0359573359,4.
6288978827,0.4566934577\H,0.4351766811,3.0699335764,1.2279256251\H,0.5
461673357,3.236755313,-0.5394085851\O,-0.4577875848,-2.4442281037,1.66
362428\H,-1.2303603932,-1.9634772147,2.0035040557\
Zero-point correction= 0.292163 (Hartree/Particle)
Thermal correction to Energy= 0.310041
Thermal correction to Enthalpy= 0.310985
Thermal correction to Gibbs Free Energy= 0.245209
Sum of electronic and zero-point Energies= -840.353697
Sum of electronic and thermal Energies= -840.335819
Sum of electronic and thermal Enthalpies= -840.334875
Sum of electronic and thermal Free Energies= -840.400651

TS-C6 (*OH)

\O,1.2826173129,3.3467986634
,0.2482986078\O,-2.7530859811,0.9905095283,0.2285588382\N,2.6726624494
,-1.9082136886,-0.5672375313\N,-3.1963285046,-1.0224657045,-0.69955756
98\C,0.4890775276,-1.5760532932,-0.1128592052\C,1.1551290398,-0.306350
889,-0.109374341\C,-0.9718933753,-1.7773261748,0.1202803104\C,2.517366
2493,-0.5459483995,-0.3739508541\C,1.4698980822,-2.5309527782,-0.35538

43443\C,-1.8063586125,-1.253351679,-1.0612624944\C,0.6788186677,1.0015
647833,0.1093107068\C,3.4425801157,0.5016928443,-0.4138491293\C,1.6002
647527,2.0334481935,0.0614973699\C,2.969516795,1.78191165,-0.193682305
9\C,-3.5603858033,0.1049626718,-0.0402398264\C,-5.0183901366,0.2220332
912,0.3432829512\C,-0.0844683381,3.6447661277,0.4897013301\H,-1.185644
3051,-2.8304537477,0.3114029538\H,-1.2678887698,-1.2162390607,1.011413
0267\H,-1.7784925461,-1.955575383,-1.8949357294\H,-1.3987413624,-0.303
7350292,-1.4067416095\H,3.5548627254,-2.3884261775,-0.5988459313\H,-0.
3741354812,1.1688745677,0.2976887725\H,4.4931712212,0.3277613479,-0.61
16427736\H,3.6394410954,2.6316649509,-0.2150777165\H,-3.8771806732,-1.
749119151,-0.8415632495\H,-5.6256309907,-0.6138000217,-0.0048422134\H,
-5.4089922015,1.1508783247,-0.0720656821\H,-5.0848636833,0.288817753,1
.4296612483\H,-0.1380312661,4.7247465999,0.5983369318\H,-0.7096333784,
3.3208617077,-0.3456828713\H,-0.4337414579,3.1611048871,1.4052464284\H
,1.3615142902,-3.5927372891,-0.4973638385\O,1.3522585746,-3.0448709021
,1.8247931416\H,1.383365508,-2.1297986636,2.1560807795\

Zero-point correction= 0.291475 (Hartree/Particle)
Thermal correction to Energy= 0.309753
Thermal correction to Enthalpy= 0.310697
Thermal correction to Gibbs Free Energy= 0.243146
Sum of electronic and zero-point Energies= -840.356518
Sum of electronic and thermal Energies= -840.338240
Sum of electronic and thermal Enthalpies= -840.337296
Sum of electronic and thermal Free Energies= -840.404847

TS-C7 (*OH)

\O,-1.344
7046267,3.1575014005,-0.0071197153\O,2.7947296475,1.0323596606,-0.0791
631845\N,-2.5229703731,-2.1712682069,-0.4984256559\N,3.269504985,-1.10
65173355,0.4785418223\C,-0.3086791757,-1.6835352968,-0.5641793292\C,-1.
0295926306,-0.4751249052,-0.3053372966\C,1.1784838037,-1.758605277,-0.
7070176101\C,-2.4036352194,-0.8310871612,-0.1396416656\C,-1.2473182697
,-2.6789495329,-0.6312475249\C,1.8687326331,-1.4683498356,0.6366426974
\C,-0.6155735068,0.8623174855,-0.2343479428\C,-3.4002194098,0.18590035
03,-0.1183202507\C,-1.5998702678,1.8291290951,-0.094529391\C,-2.985341
6166,1.4889725275,-0.0533698445\C,3.6259122138,0.1479059467,0.11093253
02\C,5.1069675946,0.4097342868,-0.0496368729\C,0.0194183352,3.56026808
64,-0.0535070381\H,1.4873834684,-2.7361954783,-1.085236342\H,1.5142617
368,-1.0058705417,-1.4262336167\H,-1.100827118,-3.7363946312,-0.793115
7036\H,1.8061758456,-2.3347064512,1.2947952641\H,1.3674422823,-0.63779
82643,1.1324912178\H,-3.2701396638,-2.7302809896,-0.1176510944\H,0.435
5408771,1.1086506124,-0.3110237598\H,-4.4501786844,-0.0735317649,-0.08
6357296\H,-3.6956172899,2.3017493916,0.0227112711\H,3.9830631648,-1.80
65533958,0.5883480838\H,5.291223553,0.7322776335,-1.0746063046\H,5.726
6784262,-0.459240445,0.1727325796\H,5.3840512489,1.2300054324,0.612578
7135\H,0.0107635618,4.6411851401,0.0539724062\H,0.5868517148,3.1049984
47,0.7605078479\H,0.4731218562,3.2825275004,-1.0069429177\O,-2.4145098
49,-1.2128995064,1.8510148123\H,-2.2712174475,-0.3156888573,2.19658301
36\

Zero-point correction= 0.291660 (Hartree/Particle)
Thermal correction to Energy= 0.309744
Thermal correction to Enthalpy= 0.310688
Thermal correction to Gibbs Free Energy= 0.244310
Sum of electronic and zero-point Energies= -840.348905
Sum of electronic and thermal Energies= -840.330822
Sum of electronic and thermal Enthalpies= -840.329877
Sum of electronic and thermal Free Energies= -840.396256

TS-C9 (*OH)

\O,1.6919420634,2.8576603677
, -0.3629209017\O,-2.5725084716,1.1717668027,-0.2908925074\N,2.39753540
62,-2.5694212402,-0.0546992725\N,-3.2975422685,-0.9642772172,-0.470303

098\C,0.2820233781,-1.8896491702,0.2885269738\C,1.1035370784,-0.745201
1842,0.0363103179\C,-1.1877163264,-1.8077632991,0.55772292\C,2.4153193
813,-1.1958478741,-0.1676414315\C,1.1125065906,-2.9808663403,0.2183625
721\C,-1.9667346808,-1.4885672398,-0.7304550504\C,0.8008534933,0.63974
03719,0.0317147871\C,3.4662754053,-0.2987489269,-0.4247991059\C,1.8499
952872,1.521761284,-0.2706564078\C,3.1691907174,1.0492129375,-0.471415
1151\C,-3.4886056331,0.3581992377,-0.2306244768\C,-4.9000333194,0.7829
25736,0.1088585174\C,0.3899799166,3.3824623442,-0.0944547732\H,-1.5605
178079,-2.7338091939,1.0029980923\H,-1.3628168509,-0.999185558,1.27366
03522\H,0.8887254674,-4.0274970208,0.3543282734\H,-2.0571961213,-2.378
3862658,-1.3550575192\H,-1.4316855292,-0.7302916933,-1.3008756291\H,3.
1915404544,-3.1757786562,-0.1575026288\H,-0.2284544075,0.9681391217,0.
0581227501\H,4.4813424002,-0.6429203664,-0.5824492343\H,3.9392266822,1
.7829817957,-0.6696212284\H,-4.0673874432,-1.5986773536,-0.3420152464\
H,-5.620861957,-0.0339209777,0.0631526026\H,-5.198277626,1.5687766915,
-0.5848131951\H,-4.8982531772,1.2075545104,1.1132446888\H,0.4950817609
,4.4617455441,-0.1634704572\H,-0.3289149389,3.0290900933,-0.8361673599
\H,0.0709339472,3.0876078217,0.9048187469\O,0.7922492875,1.1261350009,
2.1560041415\H,1.676292621,0.7463733967,2.3021223427\

Zero-point correction= 0.291459 (Hartree/Particle)
Thermal correction to Energy= 0.309733
Thermal correction to Enthalpy= 0.310677
Thermal correction to Gibbs Free Energy= 0.243850
Sum of electronic and zero-point Energies= -840.353624
Sum of electronic and thermal Energies= -840.335351
Sum of electronic and thermal Enthalpies= -840.334407
Sum of electronic and thermal Free Energies= -840.401233

TS-C10 (*OH)

\O,-1.8005267459,2.797492988
3,-0.5075612845\O,2.6004932431,1.1169343608,-0.4702534933\N,-2.3103873
226,-2.6208644914,-0.0697725139\N,3.2871297698,-0.7403709273,0.6176436
53\C,-0.1810328586,-1.9315582033,-0.284501713\C,-1.0489809333,-0.78293
06077,-0.2625081389\C,1.3095239107,-1.85861382,-0.3961837448\C,-2.3686
110434,-1.2523168024,-0.1275160922\C,-0.9927191813,-3.0273373898,-0.16
38465779\C,1.927633848,-1.2029199796,0.8511998845\C,-0.7874709934,0.59
16939701,-0.3592862473\C,-3.472558938,-0.370404065,-0.0787004581\C,-1.
8752168264,1.4837623578,-0.2136895139\C,-3.2185379915,0.972596455,-0.1
428487731\C,3.5169840496,0.4193336518,-0.0465487536\C,4.9646446913,0.8
154974517,-0.2333410543\C,-0.5047684906,3.3927034357,-0.446138714\H,1.
7383204006,-2.852328047,-0.5482400313\H,1.5777329701,-1.2469864779,-1.
2616203911\H,-0.7392248872,-4.0756402701,-0.1416180664\H,1.9419791345,
-1.9058027191,1.6846403667\H,1.3311894775,-0.3406054009,1.1504924072\H
,-3.1003369411,-3.2347367189,0.0233963689\H,0.2238046585,0.9577690485,
-0.4755384902\H,-4.4876713104,-0.7398939137,0.0011098989\H,-4.01487805
93,1.7032328492,-0.1045311302\H,4.0676300486,-1.2943926197,0.925406063
2\H,5.6680182,0.0928741287,0.1812077319\H,5.1186034072,1.7832469581,0.
24448839\H,5.1552657747,0.9362688124,-1.2997134475\H,-0.6714929749,4.4
635600212,-0.5251635748\H,-0.0320394355,3.1467111759,0.5042437703\H,0.
1161172783,3.053897558,-1.2782382852\O,-1.3685510303,1.6314298454,1.76
08483491\H,-1.6440350889,0.7572536552,2.082974996\

Zero-point correction= 0.291285 (Hartree/Particle)
Thermal correction to Energy= 0.309497
Thermal correction to Enthalpy= 0.310441
Thermal correction to Gibbs Free Energy= 0.242741
Sum of electronic and zero-point Energies= -840.348652
Sum of electronic and thermal Energies= -840.330441
Sum of electronic and thermal Enthalpies= -840.329496
Sum of electronic and thermal Free Energies= -840.397196

TS-C11 (*OH)

\O,-1.7906042587,2.716063069

7,-0.4348152794\O,2.6812839964,1.3041734276,-0.2052682407\N,-2.0370914
779,-2.7588889995,-0.1646799952\N,3.4482692838,-0.6228020737,0.6929544
317\C,0.0479343402,-1.9246515137,-0.3238625974\C,-0.8808253792,-0.8336
097855,-0.3057794859\C,1.5343774498,-1.7698393071,-0.4139245814\C,-2.1
788403259,-1.384284098,-0.2053515489\C,-0.7019784298,-3.0725378424,-0.
2355685137\C,2.1112375005,-1.1652889268,0.8772431348\C,-0.6909600435,0
.5640492374,-0.384595301\C,-3.311800314,-0.5783988579,-0.1736965966\C,
-1.8129940513,1.3662164904,-0.3456982944\C,-3.1226513062,0.8100859777,
-0.1697124567\C,3.627723382,0.6004381238,0.1349202062\C,5.0582178369,1
.0584904733,-0.0413871986\C,-0.512831217,3.3349979,-0.4792164663\H,2.0
14939084,-2.7287980737,-0.62441152\H,1.7775253545,-1.0918697909,-1.236
9307475\H,-0.3783841217,-4.1021982133,-0.2273580754\H,2.1479684687,-1.
9148072681,1.6685052816\H,1.4718242353,-0.3502396175,1.2152785303\H,-2
.7883107344,-3.4213907099,-0.0914590357\H,0.3083319399,0.9691134383,-0
.4784810676\H,-4.311255714,-0.9848682876,-0.0911530475\H,-3.9628751527
,1.4782238707,-0.2813708385\H,4.2525580929,-1.1840384124,0.9151072915\
H,5.7906359542,0.34448339,0.3360675006\H,5.1800156089,2.0093754599,0.4
72776693\H,5.2368095401,1.2328221248,-1.1026672759\H,-0.703028526,4.4
043413677,-0.5037253965\H,0.0720851647,3.0776559626,0.406406874\H,0.03
6648328,3.0328298324,-1.3738049282\O,-3.3412677569,1.1260955299,1.8805
406626\H,-2.6009889714,0.5523827822,2.1455673261\
Zero-point correction= 0.291343 (Hartree/Particle)
Thermal correction to Energy= 0.309638
Thermal correction to Enthalpy= 0.310582
Thermal correction to Gibbs Free Energy= 0.243222
Sum of electronic and zero-point Energies= -840.348721
Sum of electronic and thermal Energies= -840.330426
Sum of electronic and thermal Enthalpies= -840.329482
Sum of electronic and thermal Free Energies= -840.396842

TS-C12 (*OH)

\O,-1.3347675218,3.070812506
9,-0.115082786\O,2.8348559355,1.0481544599,-0.0264560105\N,-2.34950823
33,-2.3139558511,-0.4246911763\N,3.3557286633,-1.0462442499,0.64499615
23\C,-0.1644612085,-1.7887548865,-0.5030829777\C,-0.9367664783,-0.5791
781331,-0.3922242814\C,1.3301439666,-1.8311020392,-0.5746249051\C,-2.2
89324296,-0.9497472555,-0.3447575671\C,-1.0678135853,-2.8188852987,-0.
5059734305\C,1.961290779,-1.4416003018,0.7729991823\C,-0.5624155598,0.
776572324,-0.3232485254\C,-3.3193709611,0.0058661456,-0.1770707544\C,-
1.5722599477,1.7283638717,-0.1954217784\C,-2.9243011223,1.3536586682,-
0.1530842243\C,3.6863063489,0.2001501609,0.2275880371\C,5.1626586823,0
.4987636245,0.0930264162\C,0.0185523093,3.4918181416,-0.203063715\H,1.
679150936,-2.8210139015,-0.8791413874\H,1.6767893584,-1.1144494993,-1.
3245906571\H,-0.9001587166,-3.8821365813,-0.5784186403\H,1.899491076,-
2.2697289863,1.4794484957\H,1.4205308074,-0.5964957101,1.1983066106\H,
-3.1831790141,-2.8581204928,-0.2862923419\H,0.4849168117,1.0490056786,
-0.3577960971\H,-4.3567355109,-0.2489473968,-0.3340137544\H,-3.6689364
461,2.133470695,-0.0676814372\H,4.0851520534,-1.7197877411,0.804972206
\H,5.8015246794,-0.3309910365,0.3963764659\H,5.3926140998,1.3736523959
,0.7009578011\H,5.3696767605,0.7523260054,-0.9470301772\H,-0.004493651
3,4.5757537172,-0.1278283088\H,0.6161792142,3.0743415316,0.6107164557\
H,0.4589437686,3.1950068881,-1.1582621376\O,-3.7844675703,-0.363054242
1,1.8149388075\H,-2.9987141268,0.0701558487,2.1912560608\
Zero-point correction= 0.291141 (Hartree/Particle)
Thermal correction to Energy= 0.309509
Thermal correction to Enthalpy= 0.310453
Thermal correction to Gibbs Free Energy= 0.242436
Sum of electronic and zero-point Energies= -840.349615
Sum of electronic and thermal Energies= -840.331247
Sum of electronic and thermal Enthalpies= -840.330303
Sum of electronic and thermal Free Energies= -840.398320

TS-C4 (*OOH)

\O,2.0272

566868,2.9727169073,-0.3200699715\O,-2.1980965341,1.2189897487,-0.1702
105884\N,2.6407321454,-2.444691287,0.2739529191\N,-2.8796241558,-0.653
1843633,-1.2444879965\C,0.5189889432,-1.824486218,-0.1572204931\C,1.35
71073241,-0.6396324365,-0.1433210378\C,-0.917070867,-1.9304576063,-0.3
721671992\C,2.6706587913,-1.0698554082,0.1174887037\C,1.3614676087,-2.
8879507468,0.1177799658\C,-1.5222442818,-1.1072245858,-1.5115382255\C,
1.0923641988,0.7354186669,-0.2908964677\C,3.7428985249,-0.176129611,0.
2048104866\C,2.1552305702,1.6189344208,-0.2017773792\C,3.4726843257,1.
1661724924,0.0362663827\C,-3.1052782999,0.4408483521,-0.4814545926\C,-
4.5232335038,0.6637765985,-0.0231486123\C,0.7186846618,3.48052217,-0.5
241189382\H,-1.2629420814,-2.9663188143,-0.3761332972\H,-1.5057071766,
-1.497834677,0.7098620442\H,1.1213313341,-3.9363736436,0.2008178976\H,
-1.5432273585,-1.7041391987,-2.4259096687\H,-0.9193965503,-0.226293013
9,-1.7112789587\H,3.4368935391,-3.0252521371,0.4713131144\H,0.07922404
55,1.0831162824,-0.4288016777\H,4.7513214812,-0.5172030063,0.405560334
3\H,4.25888016,1.9071963197,0.0968506781\H,-3.6347877142,-1.3113616439
,-1.3493716517\H,-5.2537416218,0.1141557193,-0.6173497107\H,-4.7415909
565,1.7294443987,-0.0603558424\H,-4.5836141581,0.331770684,1.015523870
6\H,0.8247989174,4.560578812,-0.5801340697\H,0.292832417,3.1009348709,
-1.4565391341\H,0.059298295,3.2137083408,0.3051074248\O,-2.1252062454,
-1.0302501291,1.6770138979\O,-1.2743607434,-0.0470789014,2.1480086698\
H,-1.4913659613,0.7077762935,1.5634087235\

Zero-point correction= 0.292727 (Hartree/Particle)

Thermal correction to Energy= 0.311260

Thermal correction to Enthalpy= 0.312204

Thermal correction to Gibbs Free Energy= 0.245381

Sum of electronic and zero-point Energies= -915.485250

Sum of electronic and thermal Energies= -915.466717

Sum of electronic and thermal Enthalpies= -915.465773

Sum of electronic and thermal Free Energies= -915.532596

TS-C6 (*OOH)

\O,1.2861

68577,3.2437343836,0.3665215427\O,-2.7939816962,0.9851428421,0.2103305
506\N,2.6317106386,-2.0271500285,-0.4341541903\N,-3.2488995723,-1.0273
482322,-0.7150251925\C,0.4246571313,-1.6420024305,-0.1139651132\C,1.10
80299222,-0.4030560287,-0.0568430666\C,-1.0379122079,-1.8279180433,0.1
046506402\C,2.4857998321,-0.6642592467,-0.2456968263\C,1.4092579574,-2.
.6456142816,-0.2428999102\C,-1.8605161488,-1.2705583546,-1.0717006479\
C,0.6466643245,0.9138806117,0.1606456098\C,3.4265265303,0.3669671451,-
0.2324364742\C,1.5854847328,1.927659314,0.1716941256\C,2.9623618682,1.
6544796593,-0.0244859057\C,-3.6053526149,0.1027315543,-0.0546575216\C,
-5.0608408417,0.2229387153,0.3379034319\C,-0.0827264357,3.561445182,0.
5729301429\H,-1.2701728333,-2.8818242921,0.2713658815\H,-1.3278007234,
-1.2817612874,1.0077878524\H,-1.8361644664,-1.956613577,-1.9188026491\
H,-1.4390374061,-0.3200741679,-1.3963591045\H,3.5068300523,-2.51611958
87,-0.500922128\H,-0.4099250635,1.0954407925,0.3098127234\H,4.4830022
772,0.17863609,-0.3798473531\H,3.6459434492,2.4932746734,-0.0060370513
\H,-3.9327474251,-1.7530893945,-0.8468610984\H,-5.6791333877,-0.591207
8086,-0.0408958956\H,-5.4407447867,1.1724549396,-0.0381119963\H,-5.123
0359518,0.2461632598,1.426456315\H,-0.1206390089,4.6398469146,0.700877
5483\H,-0.6877519691,3.2649930619,-0.286943738\H,-0.4668512681,3.06605
45593,1.4676897015\H,1.2587527402,-3.6575099448,-0.5858769848\O,1.4818
06524,-3.3340819863,1.5739572003\O,1.8042881182,-2.2813435596,2.402745
5235\H,2.7709193721,-2.2254316455,2.3455614927\

Zero-point correction= 0.296203 (Hartree/Particle)

Thermal correction to Energy= 0.315537

Thermal correction to Enthalpy= 0.316481

Thermal correction to Gibbs Free Energy= 0.246564

Sum of electronic and zero-point Energies= -915.488543

Sum of electronic and thermal Energies= -915.469209
Sum of electronic and thermal Enthalpies= -915.468265
Sum of electronic and thermal Free Energies= -915.538182

TS-C4 (*OO-CH=CH₂)

\O,1.6046685589,3.268129837,
0.5332694025\O,-2.4115792157,1.7117572753,-0.0411372746\N,2.5755960894
,-1.8688036619,-1.1185535187\N,-3.1366326739,-0.1268275127,-1.15907067
28\C,0.4008124684,-1.2935949766,-1.1937930273\C,1.1701240607,-0.142301
9113,-0.7631706866\C,-1.0412029547,-1.4460971796,-1.2724669098\C,2.518
8178401,-0.5381369898,-0.7348658646\C,1.3191484662,-2.3168693271,-1.37
94591663\C,-1.8901831591,-0.3301346125,-1.8834392666\C,0.8089898452,1.
1462452397,-0.3280457351\C,3.5380366446,0.3263554802,-0.3281009849\C,1
.8216055279,2.0007947477,0.0848795146\C,3.1757524421,1.5969220023,0.07
39122967\C,-3.2426795239,0.8218245636,-0.1875123615\C,-4.4458440565,0.
6952703076,0.7160956822\C,0.2533858219,3.7067960162,0.5995570269\H,-1.
3341450137,-2.438037003,-1.6225699006\H,-1.4217204622,-1.4882822294,-0.
.0585938575\H,1.1402857292,-3.3374408493,-1.6794763157\H,-2.1232790825
,-0.5693343014,-2.9236004177\H,-1.3621015488,0.6190185672,-1.873617326
9\H,3.4140760125,-2.4192426132,-1.1840726159\H,-0.2299142459,1.4430044
662,-0.2830452645\H,4.5755896307,0.014876632,-0.3120151472\H,3.9183316
386,2.311421171,0.4045604394\H,-3.7849900194,-0.8977904956,-1.11894134
53\H,-5.2888689026,0.2062035311,0.2264462639\H,-4.7372037993,1.6867207
262,1.0556564112\H,-4.1486622219,0.1003776532,1.5831773008\H,0.2924734
698,4.721237226,0.9870039014\H,-0.2084842839,3.7022187726,-0.390315260
7\H,-0.3338878628,3.0720323573,1.2658463551\O,-1.7214761971,-1.6207463
946,1.1902041644\O,-0.6489222431,-2.352887159,1.6515804831\C,0.3430549
496,-1.5239322367,2.113792096\H,0.0890772287,-0.4732701498,2.059486289
1\C,1.4852437374,-2.0247313435,2.5744093754\H,1.6677164346,-3.09108120
37,2.5961779146\H,2.2472165813,-1.3502301162,2.9367623183\\
Zero-point correction= 0.324898 (Hartree/Particle)
Thermal correction to Energy= 0.346166
Thermal correction to Enthalpy= 0.347110
Thermal correction to Gibbs Free Energy= 0.272389
Sum of electronic and zero-point Energies= -992.834467
Sum of electronic and thermal Energies= -992.813200
Sum of electronic and thermal Enthalpies= -992.812255
Sum of electronic and thermal Free Energies= -992.886976

TS-C4 (*OO-CH₂-CH=CH₂)

\O,1.7360178202,2.620464233,
1.0985670764\O,-2.2985235532,1.3724705258,-0.1480167922\N,2.1456565976
,-2.8160944003,0.51478874\N,-2.9607091098,-0.3761930361,-1.4318811886\
C,0.1888260393,-1.9764489673,-0.2239828866\C,1.0194036219,-0.881608117
6,0.2425951506\C,-1.1765456396,-1.9520599529,-0.7204618263\C,2.2291383
851,-1.4455832152,0.6906487833\C,0.9312541284,-3.1283953997,-0.0164115
394\C,-1.6054396659,-0.8457986659,-1.6839202954\C,0.8126149915,0.50534
51172,0.360688392\C,3.2567199548,-0.6669031793,1.2315458737\C,1.827615
307,1.2744320618,0.9111712293\C,3.0443904361,0.6940682084,1.3334924764
\C,-3.1949586804,0.6431744113,-0.5630865444\C,-4.6282163013,0.81488100
25,-0.1224049906\C,0.4886855787,3.2283280414,0.791134119\H,-1.51348330
38,-2.9395849656,-1.042109547\H,-1.9245531351,-1.7980797904,0.32753202
38\H,0.6583547672,-4.1518877106,-0.2202915243\H,-1.5533277573,-1.20819
37249,-2.7130938368\H,-0.9517013269,0.0181135193,-1.6077281044\H,2.862
3295481,-3.4787517743,0.7545587361\H,-0.1295622626,0.9465276037,0.0688
440879\H,4.1851385623,-1.1095741683,1.5718244924\H,3.7984568629,1.3475
961335,1.7521060821\H,-3.72012179,-1.0150898035,-1.607455338\H,-5.3422
444427,0.4246694953,-0.848697551\H,-4.8185563659,1.8713686206,0.054911
2909\H,-4.7488785,0.2734014649,0.8188957003\H,0.6014629774,4.278434913
3,1.0469597622\H,0.2545326639,3.1276238676,-0.2712906724\H,-0.31857701
1,2.7828983816,1.3770119671\O,-2.6236538709,-1.7689234377,1.3733766498
\O,-1.6630478796,-1.7896013615,2.3608440442\C,-1.4642181604,-0.4478976

124,2.8329718845\H,-1.3989736581,0.2085593794,1.962277294\H,-2.3243309
236,-0.1551110431,3.4411720474\C,-0.1961500167,-0.4312653482,3.6269977
685\H,0.7047569288,-0.7211105304,3.0940145148\C,-0.1430868326,-0.05504
002,4.9027957516\H,-1.0384737726,0.2334825489,5.4434147631\H,0.7951540
386,-0.0152411744,5.4422335559\

Zero-point correction= 0.354071 (Hartree/Particle)
Thermal correction to Energy= 0.376648
Thermal correction to Enthalpy= 0.377592
Thermal correction to Gibbs Free Energy= 0.300124
Sum of electronic and zero-point Energies= -1032.111346
Sum of electronic and thermal Energies= -1032.088769
Sum of electronic and thermal Enthalpies= -1032.087824
Sum of electronic and thermal Free Energies= -1032.165292

TS-C1 (*OCCl₃)

\O,-2.9040484604,2.687834
9842,-0.8182685775\O,1.8311097913,1.9239529943,-0.7847929415\N,-2.3350
099124,-2.5290766162,0.7971438987\N,2.8665088115,0.3060320576,0.426265
4928\C,-0.4159442013,-1.5506351492,0.152389632\C,-1.4872904896,-0.5996
118772,0.0223684638\C,1.018263258,-1.2575942904,-0.1592648839\C,-2.670
6145697,-1.241518628,0.4322266379\C,-0.9804183914,-2.7057543876,0.6266
356729\C,1.6191120501,-0.2958329323,0.8778389636\C,-1.5132285898,0.738
8026908,-0.4166273464\C,-3.902907122,-0.5762150888,0.4194244353\C,-2.7
344080089,1.3904491117,-0.4243947886\C,-3.9186164415,0.7360550322,-0.0
093331183\C,2.8571995245,1.3854557033,-0.3776749336\C,4.1904661843,1.9
225325314,-0.8199360718\C,-1.7424014149,3.3859648004,-1.2349179542\H,1
.607335126,-2.1774340423,-0.1987474011\H,1.0872112653,-0.7798446128,-1
.1412439659\H,-0.5175405708,-3.6541888485,0.8519604388\H,1.8114768411,
-0.8152545519,1.8164388696\H,0.9153191835,0.5122570813,1.0771355848\H,
-2.975165322,-3.2295286993,1.1252269859\H,-0.5971756406,1.2242337923,-
0.7277412175\H,-4.8177908258,-1.0645502482,0.7331697965\H,-4.841318870
4,1.3007531854,-0.0389677054\H,3.7511862428,-0.075104189,0.725928794\H
,4.7160170437,1.3016770406,-1.5430585066\H,4.9789320503,1.8879597457,0
.2125299602\H,4.1452076506,2.9724449841,-1.0934182192\H,-2.0742509098,
4.3877684381,-1.4949263812\H,-1.003761487,3.4352013652,-0.4308529511\H
,-1.2906338252,2.9070169025,-2.1075465795\O,5.6930280346,1.7447931058,
1.211020841\O,5.8262903626,0.3634306555,1.2935108435\C,7.113710165,-0.
0252799858,0.9269062315\Cl,8.3186640328,0.699110875,2.0022624196\Cl,7.
4722018901,0.4192188897,-0.7588031136\Cl,7.0796411953,-1.7814025897,1.
1056019145\

Zero-point correction= 0.290583 (Hartree/Particle)
Thermal correction to Energy= 0.313880
Thermal correction to Enthalpy= 0.314824
Thermal correction to Gibbs Free Energy= 0.232337
Sum of electronic and zero-point Energies= -2333.477434
Sum of electronic and thermal Energies= -2333.454137
Sum of electronic and thermal Enthalpies= -2333.453193
Sum of electronic and thermal Free Energies= -2333.535680

TS-C3 (*OCCl₃)

\O,-2.6365054901,2.778379
5645,0.3702137557\O,3.5010620017,1.4153265407,1.0630677849\N,-2.031160
6201,-2.6732030524,0.1798478313\N,3.2895625497,-0.3161583911,-0.389406
4228\C,-0.2683499529,-1.5370728735,-0.6187072732\C,-1.2711308737,-0.59
41018307,-0.2052875949\C,1.0998995502,-1.2030063464,-1.1221284716\C,-2
.3579174953,-1.3390162663,0.2934740844\C,-0.772615809,-2.7835649418,-0
.3543284625\C,1.9800549865,-0.6648247711,-0.0012558564\C,-1.3210050878
,0.8148968537,-0.2026155459\C,-3.5072190929,-0.7154736934,0.794102532\
C,-2.4574038163,1.4258899868,0.3002044577\C,-3.5424602214,0.663551249,
0.7928147313\C,4.0085081939,0.6814393297,0.2363787332\C,5.4601597666,0
.7797776499,-0.1696340843\C,-1.5708850733,3.59735747,-0.0732330809\H,1
.566807639,-2.0909438237,-1.5605934448\H,1.0493486729,-0.4427203374,-1

.9112344554\H,-0.3093689381,-3.7494590335,-0.4831141562\H,2.0602932083
,-1.6273213321,0.7737715255\H,1.5400457239,0.12672973,0.6022926878\H,-2
.5895986309,-3.4413755598,0.5073313167\H,-0.4862925952,1.3894830028,-0
.5810511905\H,-4.3427152412,-1.2887080356,1.1774001264\H,-4.4012086618
,1.2008462335,1.1733327527\H,3.7803507301,-0.9347685253,-1.0174481005\
H,5.640036371,0.4124805985,-1.180751115\H,6.0571452477,0.1894911673,0.
5292005049\H,5.7715556198,1.8190969527,-0.0924675392\H,-1.8970514123,4
.6225821504,0.0807551002\H,-0.6643908445,3.4086710806,0.5082227334\H,-
1.3681391653,3.4331262308,-1.1354765004\O,2.2665641127,-2.8423890631,1
.3066705731\O,2.4561629052,-2.6450936563,2.6569175867\C,1.2654115521,-
2.8318242024,3.3496639083\C,1.7329186609,-2.6916283684,5.0475824342\C
I,0.0680134837,-1.5899351195,2.9282968731\C,0.5856078461,-4.448190457
3,3.0296261217\

Zero-point correction= 0.289534 (Hartree/Particle)
Thermal correction to Energy= 0.313652
Thermal correction to Enthalpy= 0.314596
Thermal correction to Gibbs Free Energy= 0.227158
Sum of electronic and zero-point Energies= -2333.489649
Sum of electronic and thermal Energies= -2333.465530
Sum of electronic and thermal Enthalpies= -2333.464586
Sum of electronic and thermal Free Energies= -2333.552024

TS-C4 (*OCCl₃)

\O,1.8149555422,3.1417859
666,-0.6142697528\O,-2.2405358027,1.4214536785,-0.3332547681\N,2.82590
48397,-2.1515292201,0.4083280167\N,-2.9138317805,-0.7368622004,-0.5266
225872\C,0.6385455641,-1.6524351132,0.2642459764\C,1.40358268,-0.44721
18401,0.0214235179\C,-0.8090799363,-1.7962936546,0.2996054552\C,2.7614
168688,-0.7967430824,0.1106796472\C,1.5676317841,-2.6535133193,0.51214
86292\C,-1.5943690605,-1.2143458051,-0.8882053913\C,1.0286758011,0.886
81096,-0.2108863154\C,3.7788378236,0.1446373215,-0.0620920259\C,2.0409
691981,1.8214927099,-0.3807133913\C,3.4026153384,1.4500366448,-0.31400
03515\C,-3.0940908413,0.5606957054,-0.1480026187\C,-4.4110987192,0.871
6121206,0.5189418107\C,0.4566116838,3.5627864289,-0.675771846\H,-1.114
2225713,-2.8207202663,0.5230698474\H,-1.2216862228,-1.194702872,1.2632
790392\H,1.3966219889,-3.6941339029,0.740298717\H,-1.6929506587,-1.987
8951687,-1.6533614345\H,-1.063051179,-0.3757486002,-1.329147929\H,3.67
28250014,-2.6814096117,0.5224004806\H,-0.01575258,1.1683041172,-0.2334
973151\H,4.8252812495,-0.1269484187,0.0046458864\H,4.1438154175,2.2256
550844,-0.45538746\H,-3.5809628053,-1.4098134596,-0.1823065554\H,-5.18
93563856,0.1478165513,0.2750804781\H,-4.7261786752,1.8711529849,0.2259
093699\H,-4.2429894493,0.8598893784,1.597773696\H,0.4893658001,4.63263
23505,-0.86244017\H,-0.0728634032,3.0565455226,-1.4856076926\H,-0.0586
371871,3.3609016148,0.2653297715\O,-1.9835996077,-0.6327885025,2.33440
58165\O,-2.9818866884,-1.5723455703,2.5317661046\C,-2.7119864648,-2.33
53721468,3.6529316019\C,1.181801316,-3.241502033,3.478851604\C,1.40
734953689,-3.4644796376,3.7454551636\C,1.6323396078,-1.3332167746,5.
1157989751\

Zero-point correction= 0.291509 (Hartree/Particle)
Thermal correction to Energy= 0.314710
Thermal correction to Enthalpy= 0.315654
Thermal correction to Gibbs Free Energy= 0.235360
Sum of electronic and zero-point Energies= -2333.493427
Sum of electronic and thermal Energies= -2333.470226
Sum of electronic and thermal Enthalpies= -2333.469282
Sum of electronic and thermal Free Energies= -2333.549576

TS-C13 (*OCCl₃)

\O,0.3389006453,-1.285522
9432,2.8233128516\O,-1.9680281627,2.2384729067,1.3338992352\N,-2.37475
63722,-3.1811740077,-1.5537649774\N,-2.7704592669,2.6731732774,-0.7340
292656\C,-2.9367918419,-1.0889121795,-0.9407910728\C,-1.9463539983,-1.

5952136497,-0.0288973773\C,-3.5065165667,0.2935513149,-0.8633505923\C,
-1.6109534874,-2.9016557659,-0.4430457572\C,-3.1627733779,-2.087213206
5,-1.8492722721\C,-2.4442127338,1.3458208838,-1.232596537\C,-1.3287763
262,-1.0239427335,1.0921011124\C,-0.656817235,-3.6637424487,0.24127460
46\C,-0.3619077794,-1.7723180886,1.7333926452\C,-0.0337038853,-3.08091
45861,1.3309071778\C,-2.5011570224,3.0185900457,0.5481761231\C,-2.8865
462359,4.418442121,0.968729838\C,0.751368923,0.0269906331,2.8079141433
\H,-4.3804327033,0.3968745361,-1.5113596509\H,-3.8321205546,0.49253094
74,0.1617519703\H,-3.8329253198,-2.1086590884,-2.6947049391\H,-2.32144
78843,1.4032023288,-2.3144410874\H,-1.4827495284,1.0639184953,-0.80356
38944\H,-2.3580517981,-4.0404557214,-2.0735775162\H,-1.5952441803,-0.0
247233324,1.4141100271\H,-0.3958996222,-4.6670331936,-0.0721514789\H,0
.7336335017,-3.6079705096,1.8822637352\H,-3.2311834185,3.3358124881,-1
.3339065513\H,-3.3417748215,5.0011806282,0.1676882722\H,-1.9904544726,
4.9284054289,1.3226634595\H,-3.5819372753,4.3478468174,1.8053545395\H,
1.0062338172,0.3323792444,3.818977137\H,1.8273194054,0.1131112661,2.19
44171452\H,0.0964560159,0.7227975099,2.2826807459\O,3.0557677165,0.302
3571725,1.6857068054\O,2.908710841,1.2568497017,0.6924308054\C,2.91383
98483,0.6550763829,-0.5544698581\C,1.5002826625,-0.4055158314,-0.7698
752133\C,2.8365172896,2.0088355425,-1.693517735\C,4.4033933147,-0.28
28940238,-0.8123132707\

Zero-point correction= 0.290194 (Hartree/Particle)
Thermal correction to Energy= 0.313048
Thermal correction to Enthalpy= 0.313992
Thermal correction to Gibbs Free Energy= 0.232853
Sum of electronic and zero-point Energies= -2333.486084
Sum of electronic and thermal Energies= -2333.463230
Sum of electronic and thermal Enthalpies= -2333.462286
Sum of electronic and thermal Free Energies= -2333.543425

TS-N2 (*OCCl₃)

\O,-3.141541603,3.2666423223,-1.0833718757\C
,-0.6327540056,-0.1542515653,1.557549522\C,-0.9775345804,1.0856285282,
0.9039185779\C,-1.4810435447,-1.3753454833,1.563164959\C,-2.1168552992
,1.4800362526,0.1995425846\C,0.1359175155,3.2075552302,0.4915831565\C,
-2.1061318508,2.7599145962,-0.3667739346\C,-0.9936441048,3.604680843,-
0.2219492048\H,-1.1208816428,-2.1054455623,2.2900898438\H,-2.507891585
2,-1.1058254598,1.8228930274\H,1.2623307123,-0.6749557743,2.6196389526
\H,-2.95428568,0.802657742,0.0903094457\H,0.9908811802,3.8643977193,0.
5864224684\H,-1.0380656934,4.5803005338,-0.6876789774\C,0.1233796746,1
.9413121238,1.0558302477\C,0.6502673011,0.0280593002,2.0776257049\N,1.
090198848,1.2786221575,1.8261824451\H,2.1324305533,1.4438777287,1.6950
5364\O,3.4023127075,1.0652536389,0.8692364259\O,3.2642970198,-0.313242
2746,0.8726674998\C,-4.2816347841,2.4343391898,-1.2613832216\H,-4.0152
690908,1.5093723928,-1.7771803088\H,-4.7406624265,2.1937184505,-0.2997
45347\H,-4.9743635786,3.0117785675,-1.8668203715\C,-1.5027299857,-1.99
94725945,0.1483443204\H,-1.5976755786,-1.2087058427,-0.5953188892\H,-0
.5730636228,-2.5333138711,-0.0448234573\N,-2.6165442972,-2.9130531109,
-0.029495612\H,-2.4654783741,-3.9060206407,0.020717493\C,-3.8634384217
,-2.4373244355,-0.2698495245\O,-4.0931650383,-1.2316386153,-0.32569986
03\C,-4.95443754,-3.4635808438,-0.4689324088\H,-5.4003587488,-3.302748
617,-1.450598116\H,-4.5983880452,-4.491393657,-0.3982322426\H,-5.72835
79487,-3.2959974438,0.2802048694\C,3.1278314046,-0.7890058329,-0.40496
84187\C,4.5951529784,-0.5123305151,-1.3723813714\C,2.857511855,-2.53
63882333,-0.1960775658\C,1.7277713208,-0.0614429442,-1.2490354759\

Zero-point correction= 0.292156 (Hartree/Particle)
Thermal correction to Energy= 0.315979
Thermal correction to Enthalpy= 0.316923
Thermal correction to Gibbs Free Energy= 0.234220
Sum of electronic and zero-point Energies= -2333.498628
Sum of electronic and thermal Energies= -2333.474805
Sum of electronic and thermal Enthalpies= -2333.473860

Sum of electronic and thermal Free Energies= -2333.556563

TS-C6 (*OCCl₃)

\O,-2.5212062212,3.351566

275,1.1384068036\O,-4.1597506706,-0.9870683621,0.7251754584\N,1.178435
7633,0.6988344598,-1.9408911823\N,-3.7032008197,-2.5391203339,-0.85251
44387\C,-0.4903939856,-0.5910418034,-1.1419286285\C,-0.7077216945,0.74
19849148,-0.700001454\C,-1.3411785109,-1.7634540437,-0.7946265697\C,0.
3575024271,1.5250178398,-1.188880834\C,0.7221209202,-0.5817009944,-1.8
566056858\C,-2.7086766568,-1.7008921501,-1.5007768852\C,-1.7192568518,
1.3116278212,0.1028315512\C,0.4532654364,2.886202441,-0.8957892302\C,-
1.6217617701,2.6613919753,0.383555415\C,-0.5431055071,3.4369993128,-0.
1112721439\C,-4.3484956397,-2.107555019,0.2603669794\C,-5.3164964391,-
3.0773532316,0.8985797915\C,-3.6100736354,2.609481906,1.6698077844\H,-
0.826755996,-2.6966424255,-1.0319652579\H,-1.516967018,-1.7498725259,0
.2848565841\H,-2.6206140145,-2.0108656225,-2.5423569149\H,-3.084618449
7,-0.6783736681,-1.4837360248\H,2.0940633983,0.9488000594,-2.272721633
5\H,-2.5276272308,0.6940300749,0.472425177\H,1.2748747478,3.4920740561
,-1.256378827\H,-0.5225708055,4.4866417125,0.1520554804\H,-3.840387524
6,-3.4855181202,-1.164337303\H,-5.4313568792,-4.0048461923,0.337307453
8\H,-6.2850683932,-2.5863260596,0.9898340035\H,-4.9622636436,-3.305836
2968,1.9043072058\H,-4.2069661801,3.3217193106,2.2326441828\H,-4.20960
26486,2.1679979222,0.8703147139\H,-3.2538816635,1.8158380456,2.3309490
291\H,1.1713554417,-1.3716832643,-2.4348422486\O,1.6811075746,-1.48140
56349,-0.1069226742\O,2.0437711018,-0.3512981585,0.6058733765\C,3.4042
703621,-0.2376283762,0.6764481955\Cl,3.6849653765,1.2791181018,1.54298
52695\Cl,4.1317727358,-1.6054539447,1.5618151366\Cl,4.1911850839,-0.15
80157811,-0.9459399759\

Zero-point correction= 0.296202 (Hartree/Particle)

Thermal correction to Energy= 0.319512

Thermal correction to Enthalpy= 0.320456

Thermal correction to Gibbs Free Energy= 0.239659

Sum of electronic and zero-point Energies= -2333.504678

Sum of electronic and thermal Energies= -2333.481368

Sum of electronic and thermal Enthalpies= -2333.480423

Sum of electronic and thermal Free Energies= -2333.561221