

Supplementary information

Cycloaddition Mechanisms of CO₂ and Epoxide Catalyzed by Salophen – A Organo-catalyst free from Metals and Halides

Cai-Hong Guo,^{*a} Min Liang,^a and Haijun Jiao^{*b}

(a) Dr. Caihong Guo; Min Liang;

Key Laboratory of Magnetic Molecules and Magnetic Information Materials (Ministry of Education), School of Chemistry and Material Science, Shanxi Normal University, Linfen 041004, China. E-mail: sxgch2006@163.com;

(b) Dr. Haijun Jiao

Leibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Straße 29a, Rostock, 18059, Germany. E-Mail: haijun.jiao@catalysis.de

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Table S1 The geometric parameters of optimized catalyst **1** were compared with the experimental molecular structure.

bond length	X-ray	B3LYP	M06-2X	bond angle	X-ray	B3LYP	M06-2X
C ₁ -N ₁	1.412	1.403	1.405	C ₁ -N ₁ -C ₂	121.39	121.13	120.15
C ₂ -N ₁	1.286	1.289	1.281	N ₁ -C ₂ -C ₃	120.42	122.40	122.21
O ₁ -H ₁	0.970	0.992	0.984	C ₄ -O ₁ -H ₁	105.70	107.42	108.04
C ₅ -N ₂	1.413	1.403	1.405	C ₅ -N ₂ -C ₆	122.70	121.15	120.06
C ₆ -N ₂	1.286	1.289	1.280	N ₂ -C ₆ -C ₇	121.05	122.40	122.24
O ₂ -H ₂	1.000	0.991	0.983	C ₈ -O ₂ -H ₂	102.60	107.50	108.14

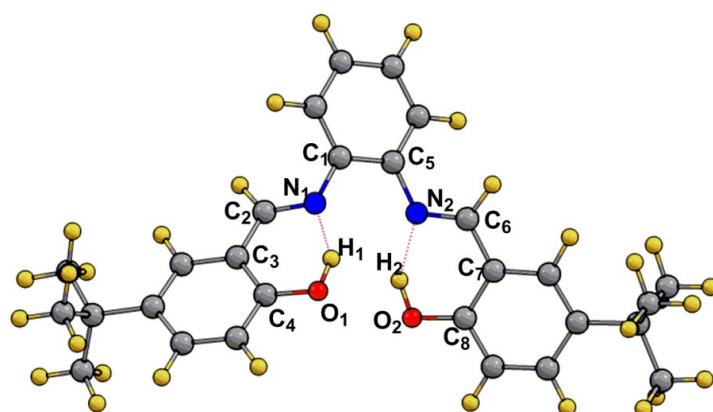


Fig. S1 Geometric parameters of catalyst **1** and its two isomers.

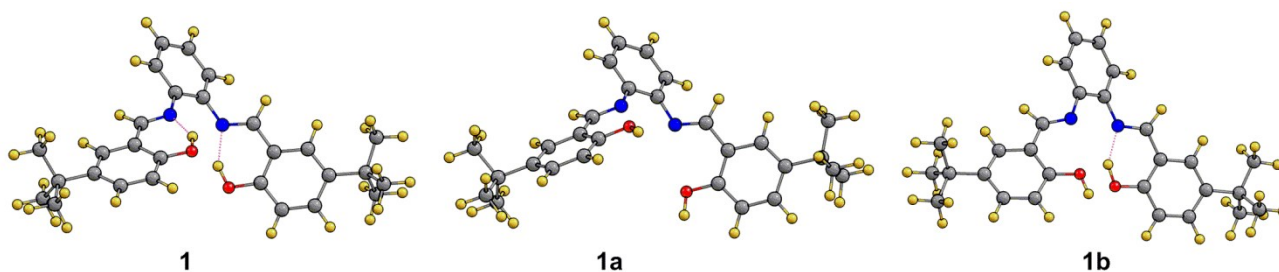


Table S2 Comparison of thermodynamic data of catalyst **1** and its two isomers.

Organocatalysts	HF(Hartree)	G(Hartree)	H(Hartree)	$\Delta G(\text{kcal/mol})$
1	-1346.870622	-1346.395641	-1346.301821	0.0
1a	-1346.825422	-1346.354015	-1346.257498	26.1
1b	-1346.850031	-1346.378032	-1346.28193	11.1

Fig. S2 Free energy profile for the dihydroxy stepwise pathway.

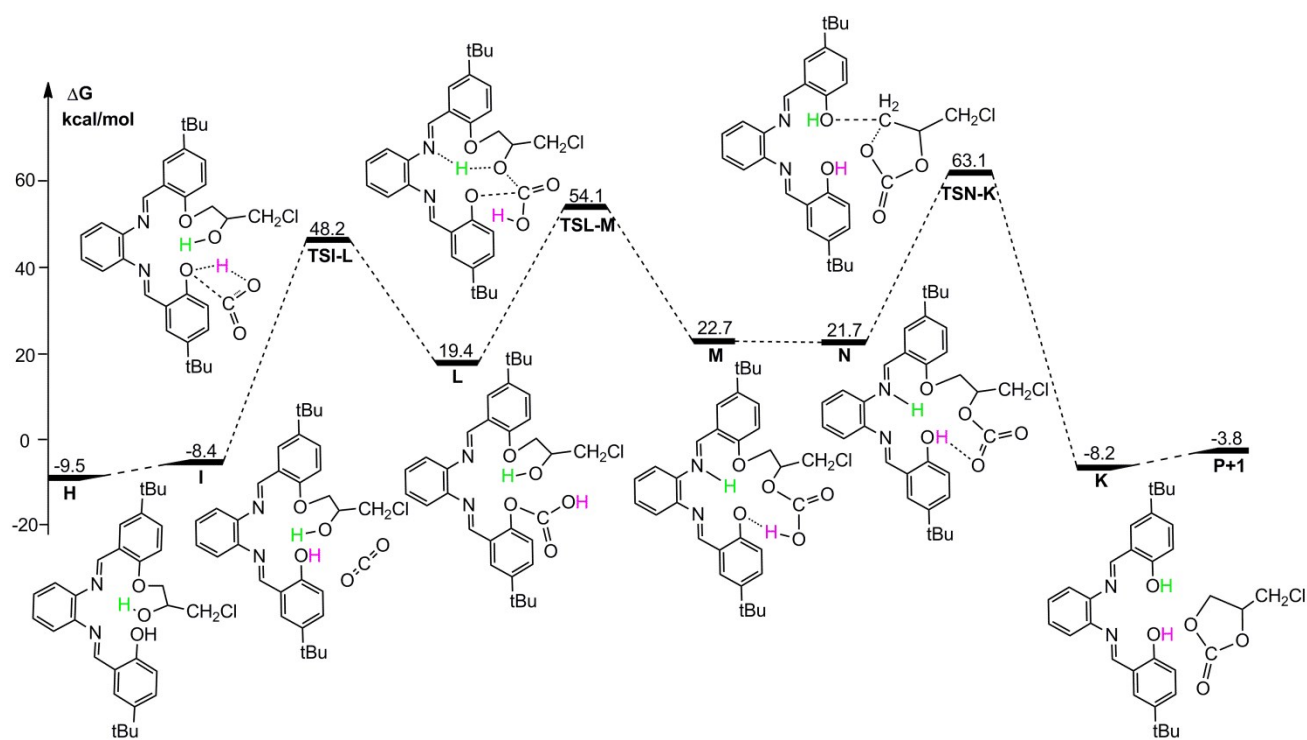


Fig. S3 Optimized structures of transition states involved in the dihydroxy stepwise pathway.

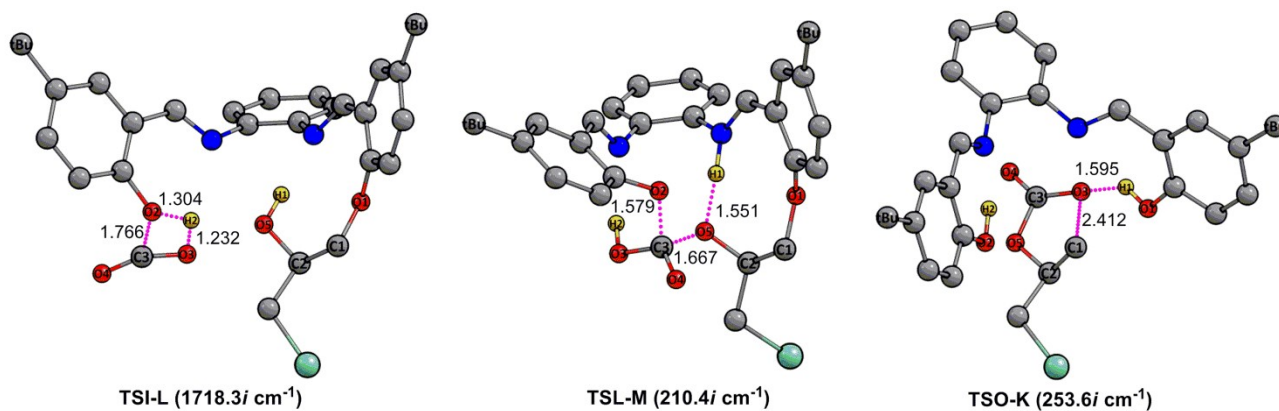
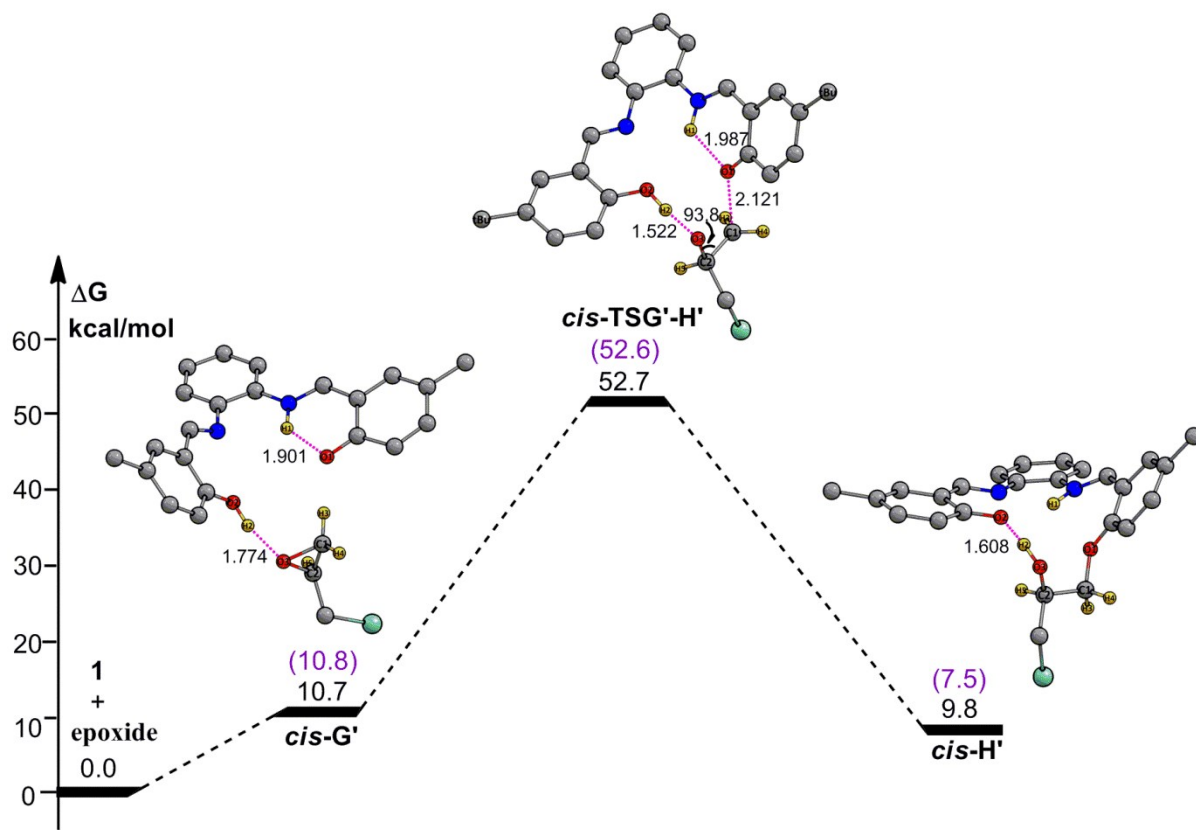


Fig. S4 Optimized structures involved in the epichlorohydrin ring-opening via the *cis*-configuration pathway.



S

Cartesian coordinates of structures at B3LYP/6-311g(d,p) level

1

C, -0.4623040408,2.7913475463,1.3522541172
C, 0.6711231046,2.3314166483,2.0174954961
C, 1.4590537933,3.2221511727,2.7396466729
C, 1.1334360646,4.5825945692,2.8112393663
C, -0.0441417718,5.0417758988,2.1718640529
C, -0.8131513751,4.1353692804,1.4310215717
H, -1.0714859461,2.1086417114,0.7712899723
H, 0.9418826106,1.2826793766,1.9777807188
H, 2.3208809961,2.8592407103,3.2875796448
H, -1.6740580758,4.5015992784,0.8838525643
N, 1.8868162673,5.4983264858,3.5611610394
N, -0.3504473485,6.409626008,2.2394997443
C, 3.1743500022,5.4348400411,3.592533536
H, 3.7201504679,4.7071348016,2.9795734855
C, -1.5703985425,6.8161671109,2.3238900893
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C, 3.9741002881,6.3181584151,4.4126349304
C, 5.3787349449,6.1919402633,4.4061214638
C, 3.3703525187,7.3130149736,5.2214320349
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H, 5.8009232415,5.4228874886,3.7703541519
C, 4.1972415116,8.1353318733,5.9971945244
C, 5.570874478,7.9762438329,5.9680392704
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Zero-point correction=	0.537518 (Hartree/Particle)
Thermal correction to Energy=	0.567857
Thermal correction to Enthalpy=	0.568801
Thermal correction to Gibbs Free Energy=	0.474981
Sum of electronic and zero-point Energies=	-1346.032802
Sum of electronic and thermal Energies=	-1346.002463
Sum of electronic and thermal Enthalpies=	-1346.001518
Sum of electronic and thermal Free Energies=	-1346.095339

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Sum of electronic and thermal Enthalpies=	-1345.957077
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1b

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Zero-point correction=	0.536204 (Hartree/Particle)
Thermal correction to Energy=	0.567156
Thermal correction to Enthalpy=	0.568101
Thermal correction to Gibbs Free Energy=	0.471999
Sum of electronic and zero-point Energies=	-1346.013375
Sum of electronic and thermal Energies=	-1345.982423
Sum of electronic and thermal Enthalpies=	-1345.981479

Sum of electronic and thermal Free Energies= -1346.077580

1-

C, 0.8390507227,4.8899948154,-0.3418998099
C, -0.5019685478,4.9736239749,0.0345370958
C, -1.2328094699,3.7995014712,0.1960722737
C, -0.6493181718,2.5430276496,-0.0061465191
C, 0.7311539824,2.4406461468,-0.3576604842
C, 1.4400137687,3.6521329027,-0.5320420507
H, 1.4202927681,5.7956875621,-0.4879116589
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C, 5.0799176467,-2.3082920874,-1.0497078729
H, 3.5576317904,-3.1322903438,-2.3069353905
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 H, -7.4209524314,0.9317642728,-0.0233655629
 H, -7.0717302897,0.3362975129,-1.6544058978
 H, -8.6321282617,-0.0068140962,-0.9020237974
 C, -7.2927221443,-2.3565030314,-1.1280104697
 H, -6.9614563504,-3.3259632828,-0.7484760333
 H, -8.3640820099,-2.4292202145,-1.3455500419
 H, -6.7641662742,-2.1703957931,-2.066748882

Zero-point correction=	0.521864 (Hartree/Particle)
Thermal correction to Energy=	0.552457
Thermal correction to Enthalpy=	0.553401
Thermal correction to Gibbs Free Energy=	0.457944
Sum of electronic and zero-point Energies=	-1345.475858
Sum of electronic and thermal Energies=	-1345.445265
Sum of electronic and thermal Enthalpies=	-1345.444321
Sum of electronic and thermal Free Energies=	-1345.539779

A

C, 0.7142430404,5.2135581211,-0.0990702591
 C, -0.6273452065,5.2027217121,0.274126578
 C, -1.2984341582,3.9920581757,0.4112555164
 C, -0.6491794606,2.7725316217,0.1775913898
 C, 0.7279427609,2.7836389618,-0.1549433977
 C, 1.3825483961,4.0119661382,-0.3099086974
 H, 1.2400523367,6.1525964364,-0.2270339898
 H, -1.1511575242,6.1329520157,0.461272743
 H, -2.3318167519,3.983445122,0.7375831614
 H, 2.4171685963,4.0187401549,-0.6327779913
 N, -1.2855659369,1.5326181952,0.3391638402
 N, 1.368509292,1.55706676,-0.3897959196
 C, -2.5252788109,1.3702647994,0.0223437938
 H, -3.1018045439,2.1776112836,-0.4450282761

C, 2.5887423313,1.3599929355,-0.0258873869
H, 3.1441614297,2.1228757272,0.5329708125
C, -3.2254076334,0.1244650242,0.2442466145
C, -4.5888650235,0.0216604807,-0.1002840503
C, -2.5624877038,-1.0014203647,0.7912924093
C, -5.3226862497,-1.1409358547,0.08397825
H, -5.0569416912,0.9023523455,-0.5235420235
C, -3.2936051797,-2.1798317166,0.9841326414
C, -4.6321877178,-2.2389150152,0.639768848
H, -2.783297756,-3.0369685618,1.4069878144
H, -5.1591821091,-3.1716673756,0.806929887
C, 3.2887591999,0.1233883339,-0.3057552488
C, 4.6208453226,-0.0335389505,0.1129678338
C, 2.6485848802,-0.9456136171,-0.9851341694
C, 5.3510409807,-1.1967788598,-0.1123202998
H, 5.0798939466,0.802136681,0.6321188065
C, 3.3666621431,-2.1204592863,-1.2120616556
C, 4.6830586041,-2.2351229049,-0.7854374623
H, 2.8688983733,-2.9383023948,-1.7184232633
H, 5.196617598,-3.1665871271,-0.9849464142
O, -1.2657431919,-0.9827275978,1.1232328104
H, -0.9211112079,-0.0747780496,0.9202315049
O, 1.3784941046,-0.8595256417,-1.4105515616
H, 1.0333370152,0.0345408263,-1.148550659
C, 6.8106828078,-1.3045997688,0.3663149051
C, 6.8700225379,-1.1123317705,1.8994596365
H, 7.9031850342,-1.1834775422,2.2534421624
H, 6.4825507237,-0.1364414213,2.2017129028
H, 6.2810234682,-1.8781470511,2.4111794704
C, 7.4321936915,-2.6731411594,0.032423012
H, 8.4645610964,-2.7034716536,0.3905360568
H, 6.892366573,-3.493563395,0.5130787389
H, 7.4520391043,-2.8597314934,-1.04481774
C, 7.6617060058,-0.2106842392,-0.3193190539
H, 7.6456649838,-0.3284005798,-1.4062189874
H, 7.2950016533,0.7921121789,-0.0873233005
H, 8.7022706163,-0.2703712252,0.0146862227
C, -6.8095017793,-1.2732972667,-0.2856728931
C, -7.6286092268,-1.6216845873,0.9786873458
H, -7.5311432146,-0.8373018361,1.7342067329
H, -8.6891623041,-1.725278438,0.7291591958
H, -7.3004015914,-2.5612776544,1.4296573754
C, -7.3782069065,0.0276455895,-0.8807502465
H, -7.3165423329,0.8595269527,-0.173442997

H, -6.858394533,0.3168454495,-1.7983709711	
H, -8.4330353223,-0.1135275571,-1.1308204452	
C, -6.9829855641,-2.3970064053,-1.3338494778	
H, -6.6408784282,-3.3627002174,-0.9542521102	
H, -8.0369908607,-2.5028957666,-1.6091287561	
H, -6.4143176867,-2.1743032561,-2.2406746877	
C, -0.6050193531,-2.7093035598,-2.2033052352	
O, -1.3256421947,-1.816364374,-2.3729503983	
O, 0.0860602973,-3.6304574059,-2.0547264573	
Zero-point correction=	0.549908 (Hartree/Particle)
Thermal correction to Energy=	0.584596
Thermal correction to Enthalpy=	0.585541
Thermal correction to Gibbs Free Energy=	0.478877
Sum of electronic and zero-point Energies=	-1534.666574
Sum of electronic and thermal Energies=	-1534.631886
Sum of electronic and thermal Enthalpies=	-1534.630941
Sum of electronic and thermal Free Energies=	-1534.737605

B

C, -0.6172511721,5.3826363282,-0.1883893465
 C, 0.7467301533,5.3453594778,-0.4692296967
 C, 1.3937418715,4.1207780326,-0.5875674607
 C, 0.6986650989,2.9135307622,-0.4336889539
 C, -0.6925541313,2.9609950909,-0.1792621136
 C, -1.3288397539,4.1980228615,-0.0384082454
 H, -1.1286797961,6.3316567719,-0.0798704433
 H, 1.303768202,6.2651208588,-0.6028969212
 H, 2.4454190333,4.087663044,-0.8460093951
 H, -2.3805193178,4.23666698,0.2168716713
 N, 1.3054017054,1.6605715722,-0.6008835498
 N, -1.3824742616,1.7468765203,-0.0433358813
 C, 2.5085547068,1.4523538038,-0.1787623638
 H, 3.0372595237,2.2180669663,0.4009952831
 C, -2.6942697547,1.5552767101,-0.1882438462
 H, -3.2900569055,2.4123441999,-0.4882092257
 C, 3.2353562055,0.230660795,-0.429796051
 C, 4.5396294627,0.0885736826,0.0893752645
 C, 2.6751608213,-0.824028249,-1.1905514208
 C, 5.3102004889,-1.044870735,-0.1182062491
 H, 4.928770863,0.9153024414,0.6714979998
 C, 3.4473138437,-1.9704467974,-1.4147831283
 C, 4.7232532029,-2.0704821231,-0.8903539245
 H, 3.0153449995,-2.7727470844,-2.0007296103
 H, 5.2824262117,-2.9786549905,-1.0863194989
 C, -3.3166779701,0.3250077322,0.0040378527

C, -4.7311496565,0.2121810766,-0.1885160343
C, -2.5230082623,-0.84239245,0.390611757
C, -5.4021920119,-0.9672956134,-0.0183024823
H, -5.2614984509,1.1126173407,-0.477447487
C, -3.2663677537,-2.0664088912,0.5580203399
C, -4.6154125284,-2.1101636248,0.3627222467
H, -2.7049823297,-2.9488951707,0.8400924858
H, -5.1180913573,-3.0617690883,0.5021834674
O, 1.4416090282,-0.7706359172,-1.7054506147
H, 1.0341490392,0.083812511,-1.4299492823
O, -1.276853205,-0.774957067,0.5616728435
H, -0.8759759563,0.8720005556,0.1927388668
C, -6.9171902632,-1.1272138645,-0.2106303596
C, -7.1908177342,-2.1595778979,-1.329603873
H, -8.268092929,-2.292839828,-1.4705382875
H, -6.760887841,-1.827171625,-2.2782923188
H, -6.7643507878,-3.1376912599,-1.0950435297
C, -7.5578157966,-1.6215763547,1.1079110368
H, -8.6376108728,-1.7488022459,0.9823882334
H, -7.1464909434,-2.5823308462,1.4261661674
H, -7.3906339514,-0.9032435219,1.915117297
C, -7.595239956,0.1969152503,-0.6046063743
H, -7.4631747947,0.963990711,0.163610564
H, -7.2064929406,0.5855984177,-1.5498880395
H, -8.6695038212,0.0377057467,-0.7305781758
C, 6.7299706063,-1.2197058507,0.4461761798
C, 7.7272088616,-1.4288203348,-0.7169216949
H, 7.7292375086,-0.5657226564,-1.3882034747
H, 8.7423299484,-1.5626978514,-0.3304424522
H, 7.4788170456,-2.3121216501,-1.3098369598
C, 7.1870370936,0.0068178229,1.2563236134
H, 7.2141176037,0.9120286471,0.6430991001
H, 6.535699609,0.1921179614,2.1148781385
H, 8.1970873817,-0.1611221046,1.6392747267
C, 6.7648180983,-2.4531013668,1.3782961396
H, 6.4922958203,-3.369111302,0.8487679256
H, 7.7697800932,-2.5929877024,1.7883987687
H, 6.0691550449,-2.3305405992,2.2126860108
C, 0.5723195824,-2.5283761371,1.6158378646
O, 1.2564155382,-1.6213285767,1.850973489
O, -0.0622780906,-3.4805522947,1.4163254326

Zero-point correction=	0.549797 (Hartree/Particle)
Thermal correction to Energy=	0.584629
Thermal correction to Enthalpy=	0.585573

Thermal correction to Gibbs Free Energy=	0.478646
Sum of electronic and zero-point Energies=	-1534.662025
Sum of electronic and thermal Energies=	-1534.627193
Sum of electronic and thermal Enthalpies=	-1534.626249
Sum of electronic and thermal Free Energies=	-1534.733176

C

C, 0.3694034592,4.8683084277,2.1663290629
 C, -0.9505686075,4.6224415292,2.5347996928
 C, -1.6180133661,3.5161218467,2.0194605585
 C, -0.9869011469,2.6395194498,1.1275130194
 C, 0.3751077379,2.8563020473,0.7990312073
 C, 1.0230039157,3.9892121241,1.3093119662
 H, 0.8904318469,5.7403837351,2.5440920147
 H, -1.4611679583,5.2877664568,3.2212564817
 H, -2.6336639176,3.3070756859,2.33442611
 H, 2.0391563173,4.1973526986,0.9956569461
 N, -1.632282669,1.5048837213,0.6038474327
 N, 0.9906630185,1.9732155663,-0.1014045687
 C, -2.8940346272,1.5294975888,0.3227769015
 H, -3.4712315145,2.4580347021,0.3991873996
 C, 2.2190679918,1.6531440816,0.0579208988
 H, 2.7868964563,2.0159049732,0.9261725355
 C, -3.6149553819,0.358194648,-0.1193392227
 C, -4.9812739724,0.4698684592,-0.4548028148
 C, -2.9797950717,-0.9044282676,-0.2163627106
 C, -5.7378846575,-0.610833583,-0.880675504
 H, -5.4303269047,1.4520443714,-0.3696058839
 C, -3.7351941333,-2.0039658209,-0.6397548938
 C, -5.0717573522,-1.8529030238,-0.9614844918
 H, -3.2437699187,-2.9665177454,-0.7127150671
 H, -5.6170708175,-2.73094996,-1.2888951537
 C, 3.0002040893,0.8138395135,-0.8562051721
 C, 4.3850190062,0.7381138527,-0.6553853872
 C, 2.4508959725,0.0812588687,-1.9248463946
 C, 5.2357036923,-0.0013368129,-1.4834017012
 H, 4.7993987259,1.2957691694,0.1778014303
 C, 3.2646149411,-0.6634113176,-2.757612172
 C, 4.6423198827,-0.6983045777,-2.541160152
 H, 2.8149209815,-1.2150272512,-3.573008492
 H, 5.2488890366,-1.2873769867,-3.2156338016
 O, -1.6845323044,-1.0850880142,0.0759461722
 H, -1.3174660567,-0.2139943343,0.3695843027
 O, 1.0782787874,0.0532282455,-2.0702225438
 H, -0.7400203967,1.085957142,-1.5969465734

C, 6.7504472986,-0.0192817727,-1.2110178062
 C, 7.0146078713,-0.5887971945,0.2022056722
 H, 8.0889172389,-0.6052512634,0.4087849099
 H, 6.5369860458,0.0113903105,0.9803106587
 H, 6.6361028914,-1.6108320157,0.2887264373
 C, 7.5136261563,-0.8869671519,-2.2280699763
 H, 8.5817059853,-0.8678141668,-1.9967194738
 H, 7.1893250467,-1.9307231465,-2.1976536158
 H, 7.3924562909,-0.5186814966,-3.2503899002
 C, 7.3038915725,1.42228406,-1.2956432584
 H, 7.129243115,1.8501998021,-2.286321748
 H, 6.8363420238,2.0812479604,-0.5601535474
 H, 8.3817595358,1.4259635455,-1.1077160554
 C, -7.224617618,-0.5074989958,-1.2598548862
 C, -8.0562768611,-1.4448483528,-0.3536172033
 H, -7.9494129401,-1.1668635902,0.698485937
 H, -9.117135236,-1.3852052798,-0.6155463777
 H, -7.7485977591,-2.4882161481,-0.4556421731
 C, -7.7675427966,0.9234774831,-1.0958485735
 H, -7.6909745733,1.2713974609,-0.0618460873
 H, -7.2408892309,1.6341839063,-1.73864216
 H, -8.8243203854,0.9490707405,-1.373982698
 C, -7.4095001713,-0.9266999314,-2.7368502444
 H, -7.0784161188,-1.9529446211,-2.9127408433
 H, -8.4643889185,-0.8643619472,-3.0214509452
 H, -6.8379954804,-0.2733284451,-3.4014002191
 C, 0.4878770556,0.8961123378,-2.9921958844
 O, 0.978852057,1.2302726404,-4.0254830541
 O, -0.7222056196,1.2310560224,-2.5595562262

Zero-point correction=	0.551580 (Hartree/Particle)
Thermal correction to Energy=	0.585072
Thermal correction to Enthalpy=	0.586016
Thermal correction to Gibbs Free Energy=	0.483877
Sum of electronic and zero-point Energies=	-1534.626145
Sum of electronic and thermal Energies=	-1534.592653
Sum of electronic and thermal Enthalpies=	-1534.591709
Sum of electronic and thermal Free Energies=	-1534.693848

D

C, -0.5754917666,4.7532044794,0.7854713191
 C, 0.7534850951,4.8850555582,0.3912872321
 C, 1.4600867079,3.7652458869,-0.0307975213
 C, 0.8614418738,2.4990634119,-0.0717067734
 C, -0.5117541012,2.3760754657,0.2542047368
 C, -1.1965144981,3.5118211383,0.713625124

H, -1.1284089164,5.6124022136,1.1473182434
H, 1.241290552,5.8524824481,0.4184095135
H, 2.4881881784,3.8704579514,-0.3562254971
H, -2.219944355,3.4048424354,1.0524999463
N, 1.5682981932,1.3553895128,-0.4813542817
N, -1.1206466671,1.1101301868,0.1878631597
C, 2.8114685149,1.2111098248,-0.1786100758
H, 3.3373329027,1.9395285229,0.4434194833
C, -2.3474501553,1.0375220727,-0.1637406422
H, -2.8974267019,1.9350246573,-0.4788404711
C, 3.5721401839,0.0540944525,-0.6155227762
C, 4.9599803447,-0.0011917706,-0.3891475709
C, 2.9355373061,-1.0393704109,-1.2395848295
C, 5.736636378,-1.0896740107,-0.7702406424
H, 5.4138616048,0.8499585082,0.1034574191
C, 3.696067005,-2.1442272255,-1.6205561016
C, 5.0636149579,-2.159297523,-1.3920555984
H, 3.1972179612,-2.9798587986,-2.0967136734
H, 5.6216457663,-3.0338340855,-1.7063405128
C, -3.1630873528,-0.1800878458,-0.1788015326
C, -4.543105452,-0.0211075464,-0.3714965522
C, -2.6771754266,-1.4890019171,-0.0202888983
C, -5.4466927072,-1.0880026102,-0.3879606004
H, -4.9090173931,0.9912924368,-0.5049394882
C, -3.5443014497,-2.565571249,-0.0433448321
C, -4.913268866,-2.3690805268,-0.2184469308
H, -3.1369860676,-3.5625728051,0.0717437541
H, -5.5578168267,-3.237611446,-0.2235181045
O, 1.5922606212,-1.0598747891,-1.4352526736
H, 1.2564212599,-0.1403419921,-1.2091261578
O, -1.3176657066,-1.7517020375,0.0469635789
H, 0.847987379,-1.7508185091,0.1165096822
C, -6.9493743824,-0.8234558903,-0.5896731959
C, -7.1719690726,-0.1260912665,-1.9516709171
H, -8.2372434229,0.0689829332,-2.1074005558
H, -6.647454599,0.8303791757,-2.0105133035
H, -6.8173753694,-0.7531422357,-2.774107471
C, -7.7743705177,-2.1230250238,-0.5755011903
H, -8.8315733166,-1.8857984032,-0.7189326217
H, -7.4779614406,-2.8028509786,-1.3789085018
H, -7.6820529434,-2.6534240261,0.3760466451
C, -7.4684034925,0.0883460667,0.5463018882
H, -7.3254245157,-0.383209359,1.5221413219
H, -6.9539550206,1.0519704226,0.5627453158

H, -8.5369509101,0.2845664689,0.416119413
 C, 7.2562412157,-1.1644972426,-0.5415135773
 C, 7.9755148009,-1.3133886299,-1.9021420562
 H, 7.7642048019,-0.4586560423,-2.5502853206
 H, 9.0583846355,-1.3708105727,-1.7554313789
 H, 7.6638718697,-2.2177924112,-2.4297606204
 C, 7.8019027417,0.0957816501,0.1536063768
 H, 7.6298570899,0.9958738624,-0.4431122933
 H, 7.3517928205,0.2450097169,1.1388669334
 H, 8.8810702065,-0.0024198435,0.2970778995
 C, 7.5857899652,-2.3861404907,0.3477625256
 H, 7.2628605528,-3.3233291777,-0.1116184601
 H, 8.6648789396,-2.4537379256,0.5164917059
 H, 7.0945146335,-2.3054756838,1.3212089799
 C, -0.6761644299,-1.6099660937,1.2507928093
 O, -1.2069513079,-1.4108139561,2.3014651453
 O, 0.6291189695,-1.7824530459,1.0724247679
 C, 1.5029466346,0.6395515163,3.7961171101
 C, 2.8053729877,0.0003920368,4.0052490682
 O, 2.6203829613,0.9331274325,2.9332040401
 H, 0.6963697823,0.072354944,3.3409496205
 H, 1.2064008911,1.4585160069,4.4458875005
 H, 3.4445151251,0.3577699899,4.8102991124
 C, 3.0559600389,-1.413321782,3.5580583365
 H, 4.06448216,-1.5325106756,3.16504677
 H, 2.3236006128,-1.7305671479,2.8204178586
 Cl, 2.9295040186,-2.5534574834,4.9747035152

Zero-point correction=	0.629620 (Hartree/Particle)
Thermal correction to Energy=	0.670198
Thermal correction to Enthalpy=	0.671143
Thermal correction to Gibbs Free Energy=	0.550624
Sum of electronic and zero-point Energies=	-2187.344521
Sum of electronic and thermal Energies=	-2187.303942
Sum of electronic and thermal Enthalpies=	-2187.302998
Sum of electronic and thermal Free Energies=	-2187.423517

D'

C, -0.6774691562,-3.1614318071,-5.2102925008
 C, 0.7157318862,-3.1233295742,-5.2199017807
 C, 1.4043599542,-2.5717988427,-4.1451908676
 C, 0.7069744023,-2.0764826988,-3.0415878759
 C, -0.7080167185,-2.135374578,-3.0068617839
 C, -1.3791097348,-2.6655560468,-4.1171171236
 H, -1.2174567167,-3.5590020926,-6.0615853213
 H, 1.2671491755,-3.4934432794,-6.0758824635

H, 2.4842741035,-2.4991141538,-4.1838864087
H, -2.462445112,-2.6561598327,-4.1282198895
N, 1.3407141527,-1.4835644563,-1.9386151027
N, -1.3471666718,-1.599053465,-1.8822332778
C, 2.6191431605,-1.5505381407,-1.5949707472
H, 3.2551731777,-2.2112013512,-2.1769138828
C, -2.4047709171,-2.1652698716,-1.4360189483
H, -2.7639197901,-3.0928302268,-1.9034872596
C, 3.1848097992,-0.8254625312,-0.537255153
C, 4.5736416427,-0.9833874585,-0.2417303324
C, 2.3742458419,0.102994295,0.2309350987
C, 5.1971675438,-0.2686551644,0.7483553739
H, 5.1285894321,-1.6972888644,-0.8397283713
C, 3.0525211946,0.8542347998,1.2419837568
C, 4.3873408518,0.6619272913,1.4774258394
H, 2.4780385511,1.5770379778,1.8114736791
H, 4.8505207298,1.2522921422,2.2610293566
C, -3.2461833107,-1.7407985754,-0.3175679746
C, -4.3633136881,-2.5639646644,-0.0609247689
C, -3.0423375029,-0.6214865614,0.5146765869
C, -5.274676831,-2.3253696318,0.9602337782
H, -4.4968182688,-3.4197640721,-0.7105844895
C, -3.9375801761,-0.3694132699,1.5540839297
C, -5.0264937634,-1.2026490078,1.763896412
H, -3.7882679438,0.4918598602,2.1864633035
H, -5.6947612082,-0.9629859232,2.5828461058
O, 1.1291257314,0.222123314,-0.0102655822
O, -1.9105389732,0.1318696228,0.321903749
C, -6.4963771557,-3.2191856628,1.230873428
C, -6.5893909346,-4.3954547261,0.2422931826
H, -7.4723029951,-4.9976452589,0.4719826304
H, -6.6860449579,-4.0515612804,-0.7912504653
H, -5.7177270784,-5.0526618935,0.3069203577
C, -6.4041122605,-3.7970976864,2.6622657238
H, -7.269907252,-4.4328934698,2.8706474306
H, -5.5008519554,-4.401316385,2.7824352893
H, -6.3812665276,-3.0083019887,3.4176108121
C, -7.7865514457,-2.3765457864,1.1011855224
H, -7.8015945934,-1.545332625,1.8097218465
H, -7.8814064849,-1.9590338218,0.0952292354
H, -8.6662734703,-2.9970290673,1.2973022202
C, 6.6856814129,-0.4104728265,1.099634638
C, 6.8284581241,-0.8571400825,2.5733997369
H, 6.3477307092,-1.8257789612,2.7348454413

H, 7.8852266776,-0.9517147035,2.8417804927
 H, 6.3747765277,-0.1408791086,3.2623527324
 C, 7.3945212412,-1.4503852583,0.2135215515
 H, 6.9541178858,-2.4453266686,0.3238664346
 H, 7.3608308287,-1.1739458617,-0.8441161991
 H, 8.4468202131,-1.5228187871,0.5007329722
 C, 7.3951904906,0.9502751899,0.9058632623
 H, 6.9649488217,1.7287475707,1.5403034971
 H, 8.4565009149,0.8660239382,1.1590348015
 H, 7.3179524879,1.2847381717,-0.1322603448
 C, -1.8827004261,1.4933913105,0.6024399854
 O, -2.8521718577,2.1555326095,0.8466121542
 O, -0.6528298442,1.937224039,0.552182124
 H, 0.049554538,1.2219751994,0.3809173527
 C, 1.1220060603,4.614115768,1.3668747606
 C, 0.2055877521,4.4233159872,2.4922725007
 O, 1.4482115727,3.6974051092,2.4214239164
 H, 0.8674657037,4.1449153361,0.4208556256
 H, -0.6859026812,3.8265618592,2.3350367543
 H, 0.1614902651,5.1751099204,3.27667169
 C, 2.0396633502,5.8022997182,1.3000151778
 H, 2.9693293226,5.5611020141,0.7870390008
 H, 2.2564249052,6.1846058522,2.2953425329
 Cl, 1.2805411455,7.1621213433,0.3552257124
 H, 0.764836122,-0.8897071871,-1.3139575823

Zero-point correction=	0.629504 (Hartree/Particle)
Thermal correction to Energy=	0.670013
Thermal correction to Enthalpy=	0.670957
Thermal correction to Gibbs Free Energy=	0.549902
Sum of electronic and zero-point Energies=	-2187.349504
Sum of electronic and thermal Energies=	-2187.308996
Sum of electronic and thermal Enthalpies=	-2187.308051
Sum of electronic and thermal Free Energies=	-2187.429106

E

C, 1.4529051222,0.6711138824,-4.251681665
 C, 2.0797399459,0.9560307023,-2.8904166704
 H, 0.8118675561,1.5096877829,-4.5301013545
 H, 2.7472699365,1.8142449037,-2.9510216917
 H, 2.6625999745,0.0927997469,-2.5533395907
 O, 0.5948233836,-0.4637672352,-4.2100593203
 C, 2.4998222193,0.4450032677,-5.345522265
 H, 1.9993755751,0.1493965759,-6.2638903652
 H, 3.223258905,-0.3205570503,-5.0609959651
 Cl, 3.4564403207,1.9431605743,-5.7268956947

C, 0.31727086,4.8809378973,2.2871626171
C, -0.9759145122,4.7859211272,2.7929368875
C, -1.6684772031,3.5804936502,2.7086611586
C, -1.0866958781,2.4548146973,2.1158098569
C, 0.2416631613,2.5427581721,1.633217996
C, 0.9202160568,3.7640113384,1.7145850941
H, 0.856244655,5.8201619733,2.3337447672
H, -1.4476206887,5.6461494614,3.2538572992
H, -2.6621989216,3.4942913298,3.1330306058
H, 1.911252359,3.8422370319,1.2824239804
N, -1.7333950892,1.2121701295,2.0603264709
N, 0.7875107307,1.4178295264,1.0025795185
C, -2.9752688318,1.1199406408,1.7341884119
H, -3.5488647938,2.0046311688,1.4330377005
C, 1.9949207311,1.0701295652,1.2036908295
H, 2.6349832149,1.5943292307,1.9276204133
C, -3.6777812672,-0.1458684105,1.7249752021
C, -5.0472991152,-0.1807727668,1.3946833079
C, -3.0070327309,-1.3557492283,2.0312724117
C, -5.7823455869,-1.3573327507,1.3675406249
H, -5.5204307505,0.7645291451,1.1570987926
C, -3.7388956522,-2.5496808593,2.0043852913
C, -5.0846243981,-2.5419209315,1.6841297986
H, -3.2219341973,-3.472600151,2.2384129308
H, -5.6108402481,-3.4901339542,1.6778438107
C, 2.6256477844,-0.0809551319,0.551003009
C, 3.9184210143,-0.4258937226,0.9936851802
C, 2.0261461017,-0.9050952552,-0.4198695198
C, 4.6151719623,-1.5476615046,0.5551839853
H, 4.3634406794,0.2257005077,1.7350785717
C, 2.6955834915,-2.0492423708,-0.8524041367
C, 3.9591089738,-2.3661433977,-0.377126088
H, 2.1915949627,-2.6968640596,-1.5606249225
H, 4.4363098391,-3.2674497639,-0.7433113582
O, -1.7070243661,-1.4000313445,2.3428538529
H, -1.3598194817,-0.4713471199,2.2872218659
O, 0.7569271102,-0.7476715529,-0.9428802527
H, 1.0611491445,-1.198402425,-3.795046626
C, 6.0210159169,-1.9174620526,1.0578831045
C, 6.5578177375,-0.9070331649,2.0874560873
H, 7.5564997606,-1.2110556468,2.4109051055
H, 6.6411390655,0.0990442272,1.6671228772
H, 5.9253856415,-0.8572669497,2.9780042366
C, 5.9760179568,-3.3109801387,1.7267485092

H, 6.9692585506,-3.5874191931,2.0927306584
 H, 5.2868448265,-3.3148464174,2.5752482174
 H, 5.6518766025,-4.0871641839,1.0296384974
 C, 6.9994021966,-1.9536120478,-0.13912664
 H, 6.697673039,-2.6889119252,-0.8889323716
 H, 7.0543942602,-0.9775461387,-0.628849929
 H, 8.0046967485,-2.2196424083,0.2008993802
 C, -7.2785449413,-1.414818731,1.0158257223
 C, -7.8551231192,-0.023968077,0.6958300278
 H, -7.3576924817,0.4343521189,-0.1633146699
 H, -8.9172602297,-0.1138056643,0.4525706879
 H, -7.7690704694,0.657510515,1.5468647656
 C, -7.4853136457,-2.3173466097,-0.22264142
 H, -6.9436618933,-1.9224209578,-1.0862644453
 H, -7.1323251207,-3.3360331237,-0.045397433
 H, -8.5473897495,-2.3735403983,-0.4815311676
 C, -8.0677296389,-1.9983642761,2.2110475333
 H, -7.9434463654,-1.3750176678,3.1007921016
 H, -9.135675507,-2.0487403007,1.9761197072
 H, -7.7352345665,-3.008248254,2.4628011913
 C, 0.2086704271,0.4286305005,-1.4165819492
 O, 1.0908639113,1.3300941496,-1.9197390784
 O, -0.9631769715,0.5954287734,-1.4008980635

Zero-point correction=	0.630965 (Hartree/Particle)
Thermal correction to Energy=	0.670948
Thermal correction to Enthalpy=	0.671892
Thermal correction to Gibbs Free Energy=	0.553347
Sum of electronic and zero-point Energies=	-2187.343070
Sum of electronic and thermal Energies=	-2187.303086
Sum of electronic and thermal Enthalpies=	-2187.302142
Sum of electronic and thermal Free Energies=	-2187.420687

E'

C, -0.6366442068,-2.1065464359,-5.2871201927
 C, 0.7553843859,-2.0631849757,-5.281218094
 C, 1.432130334,-1.6542123617,-4.1367028124
 C, 0.7280612949,-1.3088854427,-2.9813022839
 C, -0.6854959186,-1.3632640739,-2.97150663
 C, -1.3464139935,-1.7519474129,-4.1450642835
 H, -1.1701837748,-2.3952053127,-6.1851429543
 H, 1.3157353535,-2.3144318223,-6.1737356986
 H, 2.5117134991,-1.5687509938,-4.155524083
 H, -2.4297931874,-1.7401256744,-4.1593188633
 N, 1.3842097837,-0.8996653862,-1.8040668397
 N, -1.3546308698,-0.961258611,-1.8131209866

C, 2.621760575,-1.2303337502,-1.4527197123
H, 3.1243803916,-1.9517205917,-2.0903201142
C, -2.3712821413,-1.6273071925,-1.4161039725
H, -2.649532619,-2.5594953194,-1.9284064775
C, 3.3038132561,-0.732343478,-0.3400812873
C, 4.6291427235,-1.1998199558,-0.0725478906
C, 2.6865926481,0.2660245621,0.519024082
C, 5.3761352024,-0.7315570236,0.9754628323
H, 5.0317638436,-1.9504176729,-0.7432447225
C, 3.5040940882,0.7519277075,1.5962593271
C, 4.7654411319,0.2687337814,1.8028072155
H, 3.078914306,1.5120556355,2.2412205655
H, 5.3309269278,0.6677125941,2.6384064134
C, -3.2445826854,-1.3152512032,-0.2831194811
C, -4.1179978307,-2.3435805755,0.1166780976
C, -3.2924518583,-0.0889042375,0.4126125216
C, -5.0074447046,-2.2218303507,1.1793419811
H, -4.069922061,-3.2693072278,-0.4427599117
C, -4.1810847877,0.0634953619,1.4766261239
C, -5.0100322,-0.9896531585,1.8457021946
H, -4.2154310674,0.9973342141,2.0123770461
H, -5.681684592,-0.8272971962,2.6808488969
O, 1.5028636774,0.6728494793,0.3159805389
O, -2.4603473513,0.8961570494,-0.0692771003
C, -5.952826446,-3.350819181,1.6234347453
C, -5.7891637022,-4.6192988051,0.7669324035
H, -6.478374272,-5.3908031988,1.119719124
H, -6.0172118704,-4.4324043489,-0.2861682096
H, -4.7767528977,-5.027375264,0.8330443175
C, -5.6545386545,-3.7202530053,3.095033568
H, -6.3189595097,-4.5239744037,3.426466921
H, -4.6225007962,-4.0619942002,3.2108486269
H, -5.8013335277,-2.8702509753,3.7652872309
C, -7.4177386107,-2.8706007421,1.5017945904
H, -7.6101694736,-1.9933138118,2.1235326536
H, -7.6577095861,-2.6070792838,0.4681320425
H, -8.1042396323,-3.6610525399,1.8197890295
C, 6.8000316113,-1.2103136787,1.2955457319
C, 6.8295093133,-1.8322555032,2.7115267916
H, 6.1594034352,-2.6941125126,2.7711846997
H, 7.8410928128,-2.1687264524,2.9591382609
H, 6.5220117346,-1.1168498753,3.477953348
C, 7.2935281545,-2.2714759797,0.2962571316
H, 6.6623111714,-3.1644577154,0.3072186911

H, 7.3241225274,-1.8832197317,-0.7257102151
 H, 8.3076758278,-2.582122462,0.560876246
 C, 7.775187469,-0.0108413226,1.2433138065
 H, 7.5080315632,0.7648274328,1.964969324
 H, 8.7939495433,-0.3384540053,1.4722516445
 H, 7.7790672924,0.4450109893,0.24952159
 C, -2.2729511389,2.1069037158,0.5208218107
 O, -2.7734688001,2.5006154327,1.537968999
 O, -1.4447648126,2.7713724965,-0.2813519039
 H, 0.9346193202,2.0190285272,1.1879267696
 C, 0.5553925076,3.8240318705,0.5449825235
 C, -0.9210330179,4.0286026126,0.2049046935
 O, 0.6849873228,2.8841588111,1.5899028186
 H, 1.0774903323,3.4806478076,-0.3558023466
 H, -1.0590615427,4.7470657167,-0.6022971798
 H, -1.4803157186,4.3339235122,1.0894103064
 C, 1.2161912203,5.1059344037,1.0488861023
 H, 2.2475596848,4.9000924138,1.3212652038
 H, 0.6843825794,5.5127749829,1.9075810636
 Cl, 1.2643415696,6.4241239497,-0.210876162
 H, 0.8922344435,-0.2802416244,-1.1409382373

Zero-point correction=	0.633374 (Hartree/Particle)
Thermal correction to Energy=	0.672732
Thermal correction to Enthalpy=	0.673676
Thermal correction to Gibbs Free Energy=	0.557665
Sum of electronic and zero-point Energies=	-2187.373571
Sum of electronic and thermal Energies=	-2187.334213
Sum of electronic and thermal Enthalpies=	-2187.333268
Sum of electronic and thermal Free Energies=	-2187.449280

F

C, -0.7644509847,1.0264289417,-4.9483144926
 C, -1.9443184159,0.0331019736,-5.0154984727
 H, -0.4748589302,1.384966624,-5.9378105668
 H, -2.3860705269,-0.0425781911,-6.0073882139
 H, -2.7170661839,0.2532214386,-4.2787196379
 O, 0.3154158807,0.2196655487,-4.4406473575
 C, -0.9637212166,2.197384887,-4.0013341146
 H, -0.0565168452,2.7902872969,-3.9169519456
 H, -1.2859980356,1.8537407105,-3.0217852444
 Cl, -2.2565172464,3.2849616609,-4.6646612174
 C, 1.5608084358,4.1523121242,2.4333409964
 C, 0.1776660095,4.305538746,2.5051586152
 C, -0.6536921012,3.368697683,1.8983972138
 C, -0.1182104383,2.2694144221,1.2177791372

C, 1.2889194685,2.1052682691,1.1482932569
C, 2.108712008,3.0638210126,1.7615126231
H, 2.2146849688,4.889802669,2.8851145072
H, -0.2530344332,5.1626802786,3.0096883733
H, -1.7289035401,3.5076215344,1.912654367
H, 3.1843430987,2.9633202374,1.673631176
N, -0.9138590369,1.3290165426,0.5486766174
N, 1.7809392272,1.0211479287,0.4247171068
C, -2.0228182053,0.8959145774,1.0303165465
H, -2.3733856921,1.197262703,2.0251973268
C, 2.7540678645,0.3259944971,0.8763754218
H, 3.1754277516,0.5387830186,1.8713883209
C, -2.8576654856,-0.0424179572,0.2987017467
C, -4.0559377272,-0.4988685091,0.868065558
C, -2.4755941777,-0.5272273127,-0.9781670568
C, -4.900471628,-1.4082847739,0.2333063459
H, -4.3158667783,-0.1132785213,1.8489566757
C, -3.3056092542,-1.444441208,-1.6221303793
C, -4.4886242878,-1.8688172178,-1.0270748763
H, -2.9956513893,-1.8360527447,-2.5838545812
H, -5.0939902136,-2.5855594633,-1.5666579629
C, 3.3873512339,-0.8029234193,0.2011091184
C, 4.4659247113,-1.4214876879,0.8640442744
C, 2.9679476736,-1.3303206693,-1.0422170822
C, 5.1467751608,-2.5248470391,0.3624561722
H, 4.7572500656,-0.9958102854,1.8168379919
C, 3.6394589503,-2.4481326887,-1.5563682756
C, 4.6974476924,-3.0242137395,-0.8722754449
H, 3.3146005005,-2.8595529943,-2.5065766491
H, 5.1819649924,-3.8867700848,-1.3162804068
O, -1.3414529796,-0.1285136049,-1.5897969863
H, -0.8221926444,0.4250883518,-0.9430081548
O, 1.9467263337,-0.7587483063,-1.695500691
H, 1.6958070459,-1.2801502172,-2.4794692177
C, 6.3247102812,-3.1973635826,1.0879783115
C, 6.6605921064,-2.5023951834,2.4199037611
H, 7.5032725621,-3.009885777,2.8971386385
H, 6.946119767,-1.457259231,2.2718078205
H, 5.8193557628,-2.5329755398,3.1178573147
C, 5.9714180563,-4.6719826899,1.3910384883
H, 6.8027977791,-5.1673591659,1.9025102042
H, 5.0888634175,-4.7358488166,2.0332679367
H, 5.7603196168,-5.2341295347,0.4782780603
C, 7.5823282556,-3.147355876,0.1898850972

H, 7.4225132315,-3.6612632168,-0.761048271	
H, 7.8609194765,-2.1137074288,-0.0327934202	
H, 8.428809847,-3.628443395,0.6900996949	
C, -6.2009852775,-1.8682400658,0.9166557802	
C, -6.9924536192,-2.8628923581,0.0477219763	
H, -6.4203665303,-3.7725342695,-0.1541582564	
H, -7.906800228,-3.1583759226,0.5690630115	
H, -7.286290684,-2.4229736798,-0.9093081765	
C, -5.8634534843,-2.562478301,2.2564164419	
H, -5.2289340106,-3.4376503016,2.092927425	
H, -5.3359486501,-1.8916036949,2.9387367867	
H, -6.7790320696,-2.8933401984,2.7565959652	
C, -7.1049638168,-0.6437035562,1.1898542095	
H, -7.3631280016,-0.1337204404,0.2578113757	
H, -8.0340845941,-0.9567133941,1.6760983835	
H, -6.6167220562,0.0830160189,1.8436819195	
C, -0.0765403276,-1.0617295188,-4.2884492641	
O, -1.3477537107,-1.2352910792,-4.6863564088	
O, 0.6335170153,-1.9332862129,-3.8755323968	
Zero-point correction=	0.632205 (Hartree/Particle)
Thermal correction to Energy=	0.672044
Thermal correction to Enthalpy=	0.672988
Thermal correction to Gibbs Free Energy=	0.554603
Sum of electronic and zero-point Energies=	-2187.381578
Sum of electronic and thermal Energies=	-2187.341739
Sum of electronic and thermal Enthalpies=	-2187.340795
Sum of electronic and thermal Free Energies=	-2187.459181

G

C, -0.6342987477,6.5746446879,6.6364358608
 C, -0.7872510573,7.7189460798,5.7354234012
 H, 0.3688224954,6.2969922262,6.9465625494
 H, 0.1004508794,8.2468773945,5.4050758585
 H, -1.7157250557,8.283897827,5.7401044482
 O, -0.9009163346,6.3714761741,5.2413927327
 C, -1.7569768128,6.138445281,7.5348132471
 H, -1.7432598559,5.0626433339,7.7015724733
 H, -2.7213167072,6.4368402245,7.1291389351
 Cl, -1.6066549527,6.9053767172,9.1815892229
 C, 0.0999326906,3.013228699,0.1347549288
 C, 1.2549811426,2.4965997062,0.7150803778
 C, 1.9642427124,3.2580172215,1.6390032797
 C, 1.5361424279,4.5415283048,1.9995577055
 C, 0.340224491,5.0515554734,1.4395511763
 C, -0.3487371788,4.2800225776,0.4954300165

H, -0.4498909461,2.435985507,-0.5995504604
H, 1.6039935424,1.5045442242,0.4529813307
H, 2.8433079391,2.8448269433,2.1200506278
H, -1.2254984974,4.6990278999,0.0154893431
N, 2.2130679579,5.3101509936,2.9597425198
N, -0.0630429158,6.3508469094,1.7842091336
C, 3.4996667056,5.3650384062,2.9754481922
H, 4.0966706944,4.8753336477,2.196397768
C, -1.3089235919,6.6425249179,1.9242089459
H, -2.0841609287,5.8712371749,1.851087221
C, 4.231610215,6.0810169374,3.9997850785
C, 5.6399591892,6.1163535988,3.9517104176
C, 3.5579478492,6.7479385818,5.0510135571
C, 6.4056613024,6.7790631671,4.9003935966
H, 6.1175536741,5.5962881969,3.129927444
C, 4.3192239917,7.418773866,6.0146116901
C, 5.700742632,7.4293212001,5.9344117955
H, 3.8011232908,7.9288113269,6.8178599274
H, 6.2502976862,7.9629990624,6.7015291338
C, -1.7622320339,7.9914841594,2.1976009171
C, -3.1381991305,8.2574431568,2.2873152945
C, -0.839832506,9.0543439795,2.3811531184
C, -3.6492131274,9.5283744506,2.537853225
H, -3.8145371433,7.4201678556,2.1476720964
C, -1.3391051937,10.3331582162,2.6375746266
C, -2.7076871117,10.5582972438,2.7096337109
H, -0.6317985374,11.1420446609,2.7764144043
H, -3.0429321329,11.5682816991,2.9061387092
O, 2.220661842,6.7588804827,5.1576605114
H, 1.8449874466,6.2498885062,4.3907719062
O, 0.4867271514,8.8686520787,2.331557574
H, 0.6437167708,7.9096549893,2.1301330916
C, -5.1704569446,9.75804828,2.6053134926
C, -5.7834078845,8.8746368887,3.7162373532
H, -6.8663348979,9.0237811269,3.7686439343
H, -5.6034479832,7.8120479622,3.5362689198
H, -5.3584837855,9.1253849226,4.6920100214
C, -5.5235279709,11.225066612,2.9122819485
H, -6.6098732957,11.3400176611,2.9539239471
H, -5.1208306376,11.5476751613,3.8764475864
H, -5.1505367437,11.9038959759,2.1404743056
C, -5.8085153914,9.3842981762,1.2469427611
H, -5.3948418232,9.995687694,0.4404269827
H, -5.6341183193,8.3358058101,0.9933956754

H, -6.8908719899,9.5445913573,1.2752082648	
C, 7.9423706715,6.8323462538,4.8638487424	
C, 8.5129601928,6.2171677876,6.162826996	
H, 8.2045779295,5.173439987,6.2678234273	
H, 9.6068067744,6.2499066092,6.1514539312	
H, 8.1746670072,6.7560324928,7.0510538835	
C, 8.5221270882,6.0524954038,3.6698017883	
H, 8.2538626488,4.99288565,3.706694957	
H, 8.1820402738,6.4605381661,2.7139657968	
H, 9.6133217694,6.1157893204,3.6843699149	
C, 8.404799968,8.3034423173,4.7482525149	
H, 8.0586751028,8.9058393931,5.5916191441	
H, 9.4975606307,8.3589729883,4.7265985605	
H, 8.0221625297,8.7613142932,3.8321556086	
Zero-point correction=	0.615205 (Hartree/Particle)
Thermal correction to Energy=	0.653025
Thermal correction to Enthalpy=	0.653969
Thermal correction to Gibbs Free Energy=	0.538863
Sum of electronic and zero-point Energies=	-1998.744351
Sum of electronic and thermal Energies=	-1998.706531
Sum of electronic and thermal Enthalpies=	-1998.705587
Sum of electronic and thermal Free Energies=	-1998.820692

G'

C, 0.7403570147,-1.184241153,2.482573027
 C, 1.3241157066,-1.5034663198,1.1783090866
 H, -0.3121225832,-0.9156666537,2.5178458828
 H, 0.6838270161,-1.4531134682,0.3044937045
 H, 2.1843553452,-2.1666267864,1.1318522591
 O, 1.5808000682,-0.2327401744,1.8148425592
 C, 1.3304318303,-1.7167148334,3.7579484485
 H, 1.2036793411,-1.0165250082,4.5821758959
 H, 2.3855877422,-1.9500918283,3.6315534338
 Cl, 0.4976531811,-3.2538700647,4.2701120252
 C, 0.2372136902,5.4695549398,1.7913164055
 C, -1.0936262137,5.235461109,2.1289565403
 C, -1.7380787158,4.0925165414,1.667022027
 C, -1.0666958296,3.1827999715,0.8464517038
 C, 0.2866965037,3.4079085633,0.5074889746
 C, 0.9193183163,4.5588815464,0.9905725214
 H, 0.7428307985,6.3601198137,2.1455171684
 H, -1.6290786646,5.9331302084,2.7617913928
 H, -2.757363692,3.8908307284,1.9733348832
 H, 1.9433001944,4.7524461233,0.693216665
 N, -1.6721024125,2.0065386914,0.3747314139

N, 0.9155862599,2.5131852474,-0.3698398776
C, -2.9748114782,1.7874692292,0.2075288494
H, -3.6448998329,2.6238798115,0.385860987
C, 2.1034657046,2.0761324678,-0.1234378322
H, 2.6063953765,2.3212405014,0.8169274294
C, -3.4988939772,0.5602561965,-0.1955182286
C, -4.9118563433,0.4229198996,-0.3776594453
C, -2.6045774666,-0.5741981075,-0.42940978
C, -5.4913006178,-0.7540827133,-0.7662799563
H, -5.5194254463,1.3015174227,-0.1919811648
C, -3.2541831438,-1.7950529994,-0.833818852
C, -4.6077551455,-1.8659468942,-0.9891693436
H, -2.6191386882,-2.6545912426,-1.0138921168
H, -5.0355523274,-2.8142844809,-1.2979238761
C, 2.8330186622,1.2373338227,-1.04960963
C, 4.1117659902,0.773400352,-0.6965723539
C, 2.2909382978,0.8780207117,-2.3112852263
C, 4.8851343038,-0.0234447787,-1.5350580677
H, 4.487260813,1.0582767102,0.2807997193
C, 3.0599495755,0.0826227292,-3.1640161812
C, 4.3208353763,-0.3524372305,-2.7806611234
H, 2.6435089415,-0.1885417468,-4.1265918406
H, 4.8743261466,-0.9685328064,-3.4773855697
O, -1.355026107,-0.4854170085,-0.2847822608
H, -1.0937288141,1.1807941679,0.127308729
O, 1.0765480094,1.2747024273,-2.7137576747
H, 0.6745005963,1.7976574258,-1.9791000298
C, 6.2772728094,-0.5051785691,-1.0873573997
C, 6.1398130038,-1.3642805972,0.1910453232
H, 7.1218290037,-1.7133701261,0.5255682277
H, 5.6892746178,-0.799457186,1.010697664
H, 5.5129925591,-2.2408250207,0.0051856267
C, 6.9716810611,-1.3584800258,-2.1648636207
H, 7.9532554974,-1.6765196315,-1.8035631422
H, 6.4006857673,-2.2604022236,-2.4019235452
H, 7.1268999365,-0.7979869086,-3.0909135762
C, 7.1783940574,0.7148172818,-0.7876802381
H, 7.2934377294,1.3414079136,-1.6762314241
H, 6.764653904,1.3375060881,0.0090422757
H, 8.1730964736,0.3863923805,-0.4706555204
C, -7.0019420752,-0.940804992,-0.9695704067
C, -7.5222057044,-2.0339135869,-0.0066237526
H, -7.3557451453,-1.7454118088,1.034788664
H, -8.5960586387,-2.1893140175,-0.1502547287

H, -7.0242628119,-2.9925267789,-0.1703020472	
C, -7.7894351566,0.3526628882,-0.6950047794	
H, -7.660783671,0.6947703822,0.3356858121	
H, -7.4886390537,1.1614302326,-1.3667968864	
H, -8.8565106245,0.173839765,-0.8519191945	
C, -7.278439814,-1.3711644202,-2.4293905134	
H, -6.7770014187,-2.3089572184,-2.67947658	
H, -8.3516223761,-1.5168587991,-2.5874219459	
H, -6.9301122332,-0.6091420221,-3.131767643	
Zero-point correction=	0.615060 (Hartree/Particle)
Thermal correction to Energy=	0.653073
Thermal correction to Enthalpy=	0.654017
Thermal correction to Gibbs Free Energy=	0.537067
Sum of electronic and zero-point Energies=	-1998.739747
Sum of electronic and thermal Energies=	-1998.701734
Sum of electronic and thermal Enthalpies=	-1998.700790
Sum of electronic and thermal Free Energies=	-1998.817740

H

C, 1.000961268,-3.2016829124,1.8344165093
 C, 1.7471468015,-1.9236570813,2.2053283826
 H, 1.7395601686,-4.0110433618,1.7428716292
 H, 2.3432563708,-2.0644623784,3.1111294589
 H, 1.0433869645,-1.0963083382,2.3433498614
 O, 0.2900377563,-3.0352009689,0.6237339004
 C, -0.0536536741,-3.5978876397,2.8613887947
 H, -0.6048757586,-4.4612866221,2.4982248889
 H, -0.7416670765,-2.7787038383,3.056141907
 Cl, 0.6852879788,-4.0833240778,4.4540080385
 C, -0.7941642834,-2.486704979,-4.8183888919
 C, 0.5970668011,-2.5179444227,-4.8462106328
 C, 1.32258571,-2.0928794156,-3.7360601297
 C, 0.6712881588,-1.6358282705,-2.5863357826
 C, -0.7429077108,-1.5890558989,-2.5602896052
 C, -1.4555384248,-2.0226889892,-3.6846561681
 H, -1.3664919093,-2.8364562608,-5.669790521
 H, 1.1192934316,-2.8891558649,-5.7204404265
 H, 2.4052258176,-2.1478253787,-3.7344174627
 H, -2.5388871421,-2.0257797953,-3.6482862156
 N, 1.3768466255,-1.2656441848,-1.4269997471
 N, -1.3766507192,-1.1227825311,-1.396952837
 C, 2.2803898577,-0.3635556788,-1.4970183778
 H, 2.4620435403,0.1513951462,-2.4502318259
 C, -2.365644134,-0.308321885,-1.4826963746
 H, -2.6892591927,0.0842640759,-2.455524319

C, 3.0782574904,0.1548325788,-0.3818108059
C, 3.7726381549,1.3585559616,-0.6012442205
C, 3.1359917125,-0.4304797206,0.8988558431
C, 4.4688490531,2.0281655086,0.4020608617
H, 3.7270359603,1.7782985083,-1.598651361
C, 3.8127260129,0.232893939,1.9224682337
C, 4.4574722326,1.4380314195,1.6755385158
H, 3.8540066154,-0.2100396051,2.9100519259
H, 4.975284466,1.9179193926,2.4982204775
C, -3.1045656015,0.1742324781,-0.3294604784
C, -4.1517719572,1.0890042469,-0.5322654421
C, -2.7939877003,-0.2303653028,0.9933434192
C, -4.9104204009,1.6230927536,0.5058381779
H, -4.3600879563,1.3801980188,-1.5571278881
C, -3.5489492906,0.2972498075,2.0433054003
C, -4.5769700282,1.1985976543,1.8026203419
H, -3.3101347643,-0.015762281,3.0527722673
H, -5.1280679065,1.5749458306,2.6546070072
O, 2.5835312631,-1.6571195058,1.067790294
H, 0.8221547523,-2.4864119122,0.0114541951
O, -1.8112896294,-1.0942648023,1.2923553271
H, -1.3712831192,-1.4194603302,0.4727567685
C, -6.0412602701,2.6249744758,0.2100571618
C, -7.0968206528,1.9619682029,-0.7047963123
H, -7.9070591496,2.6639825372,-0.9256544867
H, -6.6651751086,1.6430418329,-1.656674767
H, -7.5311314463,1.0813732962,-0.223851354
C, -6.7486184051,3.096497149,1.4938820836
H, -7.5379670193,3.8080732741,1.2376498249
H, -7.2151790329,2.2657640059,2.0303272764
H, -6.0587569908,3.6011379479,2.1759336676
C, -5.4587028798,3.8687907128,-0.5002206046
H, -4.7099249598,4.3603474673,0.1267713494
H, -4.9811958631,3.6081006386,-1.4478249948
H, -6.2515648496,4.5920556971,-0.7152770258
C, 5.2160468493,3.3530560944,0.1702466961
C, 6.710152088,3.17049842,0.5244509081
H, 7.1671609271,2.3973857786,-0.0990725372
H, 7.2554279639,4.1051852719,0.3621543437
H, 6.8486515138,2.8823513983,1.5690846683
C, 5.1250039001,3.8249693967,-1.2921700522
H, 5.5645474277,3.0991341247,-1.9820019853
H, 4.091394769,4.0086424658,-1.5980140665
H, 5.6732751925,4.7634040491,-1.4093251642

C, 4.6055272464,4.4512017499,1.0714742243	
H, 4.6784153926,4.1936220502,2.1306497355	
H, 5.1294865943,5.4002453846,0.9226909344	
H, 3.5487519887,4.6055757117,0.8374191328	
Zero-point correction=	0.617728 (Hartree/Particle)
Thermal correction to Energy=	0.654496
Thermal correction to Enthalpy=	0.655440
Thermal correction to Gibbs Free Energy=	0.546113
Sum of electronic and zero-point Energies=	-1998.763697
Sum of electronic and thermal Energies=	-1998.726928
Sum of electronic and thermal Enthalpies=	-1998.725984
Sum of electronic and thermal Free Energies=	-1998.835312

H'

C, -0.0504552805,-2.5384123185,1.2760587283
 C, 0.8458447554,-1.4279800882,1.8577090917
 H, -0.5002318544,-2.1533655875,0.3539066401
 H, 0.1789547576,-0.7478545811,2.3814755534
 H, 1.5964764675,-1.8124807871,2.5509508121
 O, -1.0254577899,-2.8186486414,2.2566534274
 C, 0.6008514052,-3.8871652102,0.9916630929
 H, -0.183570442,-4.6152994804,0.8070106082
 H, 1.2209256146,-4.2255583664,1.8211954845
 Cl, 1.6551444438,-3.8907389026,-0.4959840275
 C, -0.9342053667,5.4655172455,-0.6875535836
 C, 0.4584520515,5.4941657771,-0.8472555688
 C, 1.1854150885,4.3272949452,-0.6896143156
 C, 0.530855598,3.1233583296,-0.4051036872
 C, -0.8845861817,3.0614243715,-0.2559269662
 C, -1.5866453531,4.2856740318,-0.3842444222
 H, -1.5038772216,6.3839458678,-0.7753751054
 H, 0.9688436742,6.4260126251,-1.056316542
 H, 2.2658524349,4.3654453918,-0.7574634032
 H, -2.6543817673,4.2921927952,-0.2072569721
 N, 1.2220710949,1.9116596113,-0.2135632795
 N, -1.4465267666,1.8531853709,0.0630810847
 C, 2.4828525632,1.6739374223,-0.4820363754
 H, 3.0081873553,2.4719674967,-0.9943086342
 C, -2.6892691898,1.6238963934,-0.2843161956
 H, -3.1617632288,2.3334914693,-0.9777154449
 C, 3.269810368,0.5321463358,-0.1441179074
 C, 4.6395891445,0.5714901097,-0.5078202327
 C, 2.7835054859,-0.5795208081,0.5940976869
 C, 5.5386682647,-0.416146394,-0.1470077142
 H, 4.9737956671,1.4288748016,-1.0783543094

C, 3.6884761885,-1.5695812142,0.9840073317
C, 5.0221829918,-1.4812955306,0.6188447934
H, 3.3482518911,-2.4287133091,1.5416816935
H, 5.6808404303,-2.2828946093,0.931835717
C, -3.5413718694,0.5454447376,0.0669428897
C, -4.8071567178,0.518915955,-0.5861239338
C, -3.2090708119,-0.4991059235,1.0271306666
C, -5.7540267329,-0.4636130804,-0.4004842534
H, -5.0132008759,1.3335372301,-1.2755314806
C, -4.2077768149,-1.5256302481,1.176451421
C, -5.4044929513,-1.5017895566,0.5083783783
H, -3.9799426609,-2.335449983,1.8610695224
H, -6.1025951114,-2.3104683091,0.6899370634
O, 1.4691250625,-0.5814700386,0.8510488346
O, -2.1313347523,-0.5237592147,1.6902157892
H, -1.6120536162,-2.0129471834,2.2399706909
C, -7.1005776953,-0.4165944917,-1.1470520024
C, -6.855724993,-0.4257680725,-2.67397341
H, -7.8061030178,-0.393982966,-3.2174403882
H, -6.260716667,0.4339982347,-2.9911411182
H, -6.3199467936,-1.3300568073,-2.9752594929
C, -7.9978602311,-1.6209287537,-0.8044455523
H, -8.9400068812,-1.5463226996,-1.3549489308
H, -7.5280169252,-2.5690107704,-1.0807165269
H, -8.2400503758,-1.657828045,0.2611975686
C, -7.8649209255,0.8721542906,-0.7643180947
H, -8.0620176297,0.901788561,0.3107956585
H, -7.294581712,1.7680535869,-1.0217809063
H, -8.8246655763,0.9234025493,-1.2896318745
C, 7.0264408824,-0.3918073563,-0.5330146204
C, 7.3597718958,-1.6512831167,-1.3660395211
H, 6.763507939,-1.683842221,-2.2816724323
H, 8.4167154206,-1.6492552583,-1.6479740666
H, 7.1676764116,-2.5715670104,-0.8095717511
C, 7.3879068133,0.8485270105,-1.3696493831
H, 6.8292307604,0.8838032517,-2.3091929367
H, 7.2051602235,1.7779821586,-0.8227617669
H, 8.4507497454,0.8218876878,-1.6217211449
C, 7.8900257095,-0.3790672615,0.7495455909
H, 7.7114151009,-1.2600580376,1.370450885
H, 8.9525887388,-0.3678828063,0.4899580381
H, 7.6786460015,0.5061655003,1.35546364
H, 0.6355313388,1.1681458949,0.1884838921

Zero-point correction=

0.618283 (Hartree/Particle)

Thermal correction to Energy=	0.654808
Thermal correction to Enthalpy=	0.655752
Thermal correction to Gibbs Free Energy=	0.547699
Sum of electronic and zero-point Energies=	-1998.725017
Sum of electronic and thermal Energies=	-1998.688492
Sum of electronic and thermal Enthalpies=	-1998.687548
Sum of electronic and thermal Free Energies=	-1998.795600

I

C, 1.1316591187,3.3776292853,-1.0650274631
 C, 1.822075897,2.1487712419,-1.6444657998
 H, 1.9020774271,4.1282909336,-0.8409935829
 H, 2.4168325297,2.4131148981,-2.5226981869
 H, 1.0841441503,1.3841071072,-1.9081338594
 O, 0.4136995238,3.0391974089,0.1113743183
 C, 0.0982770603,3.9837101037,-2.0084886622
 H, -0.4050104011,4.808229504,-1.5121358113
 H, -0.6268463527,3.2387897445,-2.3271205701
 Cl, 0.8681161594,4.6748591737,-3.5082886153
 C, -0.9379702374,1.2989436508,5.2486703716
 C, 0.4518435788,1.2935498991,5.3228261361
 C, 1.207098899,1.1027971854,4.1688157428
 C, 0.5869204459,0.9185917317,2.9296088572
 C, -0.8252669348,0.9078032928,2.8536153323
 C, -1.5682728972,1.1042208506,4.0233490064
 H, -1.5326386501,1.4713126871,6.1382454379
 H, 0.9502470631,1.457596188,6.2711901893
 H, 2.289829188,1.135107278,4.2098853963
 H, -2.6494338519,1.1413669662,3.9570338699
 N, 1.328240247,0.790361702,1.7393122758
 N, -1.4255833537,0.7131347632,1.5986067592
 C, 2.2054091484,-0.1354661686,1.6447279863
 H, 2.3314130708,-0.8485308284,2.4705473898
 C, -2.4448017416,-0.0598101154,1.4781381538
 H, -2.8272336056,-0.6272046045,2.3362616097
 C, 3.0437623932,-0.4278522208,0.4781010548
 C, 3.705250473,-1.6699332942,0.4665038522
 C, 3.1778082232,0.4143585329,-0.6426959477
 C, 4.4434444397,-2.1276925944,-0.621992607
 H, 3.6005179974,-2.2922000792,1.3468359654
 C, 3.9006558957,-0.0308637948,-1.7491959109
 C, 4.5132071747,-1.2769891562,-1.7365033409
 H, 4.0033862387,0.6146008221,-2.6130287052
 H, 5.0708633416,-1.5812006988,-2.6148422338
 C, -3.1404292215,-0.2639295906,0.2201429788

C, -4.23654553,-1.1417565009,0.1825630201
C, -2.7354590507,0.3802747008,-0.9760992383
C, -4.9554559008,-1.4132377772,-0.9787099209
H, -4.5179113744,-1.6198582716,1.1156232076
C, -3.4462405935,0.1148596027,-2.1479554897
C, -4.5260330922,-0.7582986875,-2.1448146181
H, -3.1347984388,0.6092506087,-3.0604146915
H, -5.0418863297,-0.9261012612,-3.0812543155
O, 2.6548833382,1.6657497447,-0.5772669649
H, 0.8889614406,2.3271948987,0.589976868
O, -1.6998128098,1.2333690464,-1.0347571207
H, -1.3121259153,1.3510985361,-0.1343783312
C, -6.1499135752,-2.3840335852,-0.9470559114
C, -7.2271180458,-1.8494833901,0.0249154128
H, -8.0820025491,-2.5319840161,0.0602705666
H, -6.8405138758,-1.7482294046,1.0418513992
H, -7.5877150443,-0.8679580715,-0.2943097102
C, -6.7975360067,-2.5529644011,-2.333675556
H, -7.6383487973,-3.2481132288,-2.2635550944
H, -7.1849640261,-1.6066185049,-2.7209551363
H, -6.093297273,-2.960207231,-3.0643681943
C, -5.6749051365,-3.7753524131,-0.4676495134
H, -4.9131193711,-4.179879461,-1.1396140128
H, -5.2458072606,-3.7339011196,0.5364546467
H, -6.5138543363,-4.4777465569,-0.4414046752
C, 5.1571211023,-3.4903237091,-0.6451172198
C, 6.6727924137,-3.2735089414,-0.8620978552
H, 7.1023864918,-2.6778286302,-0.052127793
H, 7.1935195708,-4.2353939893,-0.8904836809
H, 6.8793129045,-2.7568211242,-1.8022619425
C, 4.9676316881,-4.2709260043,0.6681433756
H, 5.3705811526,-3.7272845258,1.5271191645
H, 3.9146090778,-4.4919952071,0.8630729196
H, 5.4970379366,-5.2252009372,0.6061840357
C, 4.5913889513,-4.3471692942,-1.8014011765
H, 4.7369578982,-3.8668278526,-2.7717134946
H, 5.0919568905,-5.3196267886,-1.8334691289
H, 3.5197088544,-4.5198517966,-1.6711411087
C, -0.3605005941,5.1967020246,1.7793551324
O, -0.3669670298,4.5300381742,2.7277941956
O, -0.3672579913,5.9104011709,0.8622666731

Zero-point correction=	0.630300 (Hartree/Particle)
Thermal correction to Energy=	0.671383
Thermal correction to Enthalpy=	0.672327

Thermal correction to Gibbs Free Energy=	0.550376
Sum of electronic and zero-point Energies=	-2187.397546
Sum of electronic and thermal Energies=	-2187.356463
Sum of electronic and thermal Enthalpies=	-2187.355519
Sum of electronic and thermal Free Energies=	-2187.477470

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C, -1.0025949595,-2.2365883548,1.0998360026
 C, -1.4438884024,-1.9062696504,-0.3316081153
 H, -1.8723940062,-2.270433279,1.7635528104
 H, -0.5797109669,-1.8860452025,-0.9906514987
 H, -2.187523529,-2.603066373,-0.721860927
 O, -0.1501390029,-1.2387039158,1.601055936
 C, -0.2908208525,-3.5901461867,1.1595432862
 H, 0.08581255,-3.7565216947,2.1650801908
 H, 0.5238799981,-3.6357265186,0.4400599717
 Cl, -1.418550353,-4.985836931,0.7907129425
 C, 1.4102756783,5.1143921644,-1.5959838673
 C, 0.0310240016,5.3560762105,-1.6098169349
 C, -0.8385457597,4.3484809829,-1.227359541
 C, -0.3407799034,3.1126690059,-0.8012400178
 C, 1.0556795846,2.8434149416,-0.7668678111
 C, 1.9088618141,3.8855239063,-1.2022340003
 H, 2.0950822571,5.8867933601,-1.9278674706
 H, -0.3582403985,6.3057556481,-1.9549410108
 H, -1.9070895621,4.5110520662,-1.3027922608
 H, 2.9730743027,3.6964091196,-1.2570183926
 N, -1.1987418021,2.0615567789,-0.4137856956
 N, 1.4631781938,1.5855006526,-0.3919981591
 C, -2.4417375119,2.1876410149,-0.0233155018
 H, -2.7924789999,3.2081196305,0.0862735198
 C, 2.6634461642,1.4277660139,0.1081473844
 H, 3.2258914024,2.329437493,0.3864980302
 C, -3.3904115154,1.1650484288,0.2808791351
 C, -4.6509050823,1.5838398644,0.7734100127
 C, -3.137576014,-0.2227324668,0.1214151795
 C, -5.6504799218,0.6937914589,1.12589976
 H, -4.8113452647,2.6495263328,0.8778044041
 C, -4.1409237372,-1.1314780084,0.4731635343
 C, -5.3558093799,-0.6749332513,0.9601031515
 H, -3.9749070655,-2.1943742257,0.3692176898
 H, -6.1019644628,-1.4167925959,1.2201633477
 C, 3.3827405501,0.2260866477,0.346964102
 C, 4.7070777551,0.3838676354,0.8547841354
 C, 2.8815625738,-1.1031142962,0.0512279982

C, 5.578766962,-0.661144415,1.0520050787
 H, 5.0225445007,1.3974212624,1.0763793024
 C, 3.8258807969,-2.1695130446,0.2363514363
 C, 5.0925835078,-1.957060649,0.7116479466
 H, 3.4848487403,-3.1692737951,-0.0095017854
 H, 5.7454629632,-2.8158166818,0.8344307986
 O, -1.9477810277,-0.5498094505,-0.39369366
 O, 1.6892910289,-1.3407918737,-0.3284746517
 H, 0.5797260331,-1.1294791016,0.9406643076
 C, 7.0093736798,-0.496635746,1.5876714415
 C, 7.1785348175,-1.3226099033,2.8843707883
 H, 8.1967067772,-1.22112293,3.2741386855
 H, 6.4817133747,-0.9812559965,3.6546932834
 H, 6.9927332578,-2.3858810943,2.7149451847
 C, 8.0208812201,-0.9987095943,0.5303431931
 H, 9.0463952158,-0.900954215,0.9016837054
 H, 7.8567371694,-2.0497895359,0.280395818
 H, 7.9352610819,-0.4205251992,-0.3937669854
 C, 7.3445713051,0.9705940425,1.9110566123
 H, 7.2801142974,1.6061481499,1.0234695605
 H, 6.6764571153,1.3791288334,2.6744069259
 H, 8.3668377503,1.0406676096,2.2934619606
 C, -7.0178019238,1.1289001284,1.6782272139
 C, -7.2141493262,0.5271659066,3.0893171455
 H, -6.439127521,0.8777071397,3.7760047841
 H, -8.1865145131,0.8225859259,3.4939624238
 H, -7.1797563956,-0.5647063282,3.0759602009
 C, -7.1383189661,2.6595841474,1.7868569937
 H, -6.389361068,3.080451134,2.4635326468
 H, -7.0390971372,3.1472106601,0.8128414756
 H, -8.1218251658,2.9212793461,2.1845267027
 C, -8.1375436104,0.6200799777,0.7412202713
 H, -8.132915477,-0.4688083491,0.6527906514
 H, -9.1171263441,0.9160329555,1.1275957677
 H, -8.0279625052,1.0379686863,-0.2631074883
 H, -0.7644351154,1.1305482512,-0.4239371646
 C, 1.2905852904,-0.2019540967,-2.9097256674
 O, 2.4317573122,-0.1036471972,-3.0846575207
 O, 0.133311527,-0.2845723665,-2.8218727042

Zero-point correction=	0.631513 (Hartree/Particle)
Thermal correction to Energy=	0.672125
Thermal correction to Enthalpy=	0.673069
Thermal correction to Gibbs Free Energy=	0.553938
Sum of electronic and zero-point Energies=	-2187.368770

Sum of electronic and thermal Energies=	-2187.328158
Sum of electronic and thermal Enthalpies=	-2187.327214
Sum of electronic and thermal Free Energies=	-2187.446345

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C, -1.2929233019,-2.6787853265,-1.7842902096
 C, -1.6206407476,-1.2003148145,-1.6351510119
 H, -2.2017247793,-3.2241327928,-2.0546771837
 H, -1.7442374921,-0.7421892944,-2.6196232508
 H, -0.8348501395,-0.6925299928,-1.0755094971
 O, -0.7319676564,-3.2262674078,-0.5729648964
 C, -0.205556035,-2.9419003735,-2.8248763431
 H, 0.0747161427,-3.990734172,-2.7951489201
 H, 0.6647689002,-2.3138091955,-2.6521596569
 Cl, -0.7992072666,-2.6048574009,-4.5100267378
 C, 0.5543659427,-1.8848028304,4.9896186725
 C, -0.8356682598,-1.8116919186,4.9814465251
 C, -1.4991547568,-1.3508708752,3.8488194149
 C, -0.7896909962,-0.9622407112,2.7060549842
 C, 0.622410098,-1.0380893169,2.7140830433
 C, 1.2745227086,-1.4990329566,3.8635822462
 H, 1.0777594836,-2.2644388262,5.8592919564
 H, -1.4059926534,-2.133873024,5.8447611882
 H, -2.5822079171,-1.3354093834,3.8184286684
 H, 2.3539725428,-1.5955292674,3.8495104138
 N, -1.4485457086,-0.5425875803,1.5383728513
 N, 1.3249635219,-0.6728272303,1.5548923774
 C, -2.3395577395,0.366626822,1.621561671
 H, -2.523634646,0.886066202,2.5723813549
 C, 2.3926193044,0.0410022552,1.620279569
 H, 2.7422758648,0.4500038105,2.5758895375
 C, -3.1650904883,0.8475723078,0.5051716895
 C, -3.8115922591,2.0854804026,0.6773785046
 C, -3.3754730876,0.1573926852,-0.6995739668
 C, -4.6140147435,2.671066323,-0.2999874638
 H, -3.6548513985,2.5938104952,1.6204749968
 C, -4.1868163342,0.7130626584,-1.683313185
 C, -4.786161012,1.9511978382,-1.4919796353
 H, -4.354977498,0.151052375,-2.5946453372
 H, -5.4088105614,2.3502464236,-2.2839413727
 C, 3.1817713622,0.363318093,0.4452864016
 C, 4.3197421566,1.175416862,0.5714153689
 C, 2.8186296195,-0.1190073567,-0.837590021
 C, 5.1190232194,1.5316923292,-0.5127113319
 H, 4.5690382095,1.5294270329,1.5668479725

C, 3.6096314653,0.2285626578,-1.9318979162
 C, 4.7293160913,1.0347906895,-1.7674258079
 H, 3.3321687386,-0.1430866982,-2.9110883523
 H, 5.3101160762,1.2758780693,-2.6480779219
 O, -2.8697034904,-1.1110042949,-0.9134392157
 H, -2.9057951711,-2.5560840171,0.0636324046
 O, 1.7410509266,-0.9030388749,-1.0256564277
 H, 1.3230231767,-1.0599759386,-0.1353972111
 C, 6.3554121208,2.4262670833,-0.3085911584
 C, 7.3412220203,1.7343213259,0.6611148921
 H, 8.2246467753,2.3607871753,0.818650589
 H, 6.8872079338,1.5488778781,1.6375710026
 H, 7.6726325415,0.7730683905,0.2593223469
 C, 7.0977138771,2.7008099132,-1.629131342
 H, 7.9637880531,3.3396190106,-1.4372438412
 H, 7.4645201707,1.778932765,-2.0888558995
 H, 6.4623734286,3.2168697749,-2.3541601202
 C, 5.9187740703,3.7840525495,0.2889782748
 H, 5.2239881686,4.2992540975,-0.3798589305
 H, 5.4228278888,3.6612699691,1.2548825898
 H, 6.7878271674,4.4314191014,0.4416560683
 C, -5.2988549838,4.036426881,-0.116574072
 C, -6.8303995786,3.8661734856,-0.2474308951
 H, -7.2149419816,3.1851037811,0.5164989688
 H, -7.3297678438,4.831765447,-0.1248748935
 H, -7.1142476486,3.4677495561,-1.2240719669
 C, -5.0001565892,4.6600502498,1.258710548
 H, -5.3617032424,4.0329358997,2.0783289066
 H, -3.9304972025,4.8345009233,1.4036683147
 H, -5.5037011294,5.6267907994,1.3392644328
 C, -4.7952354238,5.0091801789,-1.2081662166
 H, -5.0149335516,4.6415715782,-2.2131359089
 H, -5.2782021703,5.9845681468,-1.0975858373
 H, -3.7141605836,5.1544834155,-1.1339173888
 C, -1.5024807649,-3.8419090603,0.3866620785
 O, -2.7746996565,-3.4392707996,0.4671695037
 O, -1.0254005179,-4.6808490574,1.0859715754

Zero-point correction=	0.632643 (Hartree/Particle)
Thermal correction to Energy=	0.672034
Thermal correction to Enthalpy=	0.672978
Thermal correction to Gibbs Free Energy=	0.557609
Sum of electronic and zero-point Energies=	-2187.367649
Sum of electronic and thermal Energies=	-2187.328258
Sum of electronic and thermal Enthalpies=	-2187.327314

Sum of electronic and thermal Free Energies= -2187.442682

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C, 0.7789729127,-1.2272890814,1.3354536425
C, -0.362449437,-1.7227577579,0.4264513213
H, 0.7796215901,-0.1327666495,1.2827982757
H, 0.015081651,-2.0080939659,-0.5513150415
H, -0.9248419371,-2.5366143405,0.8700551769
O, 2.05111169415,-1.6275483432,0.9073359507
C, 0.5966607554,-1.6318038282,2.800513754
H, 1.4225887153,-1.2513744971,3.3949040963
H, 0.5129672462,-2.7101197702,2.8935230041
Cl, -0.9294742028,-0.9127890672,3.5388693668
C, 0.1091068411,5.8169175829,0.923736036
C, -1.2324181333,5.6278801989,1.2596519366
C, -1.8255005357,4.3879641922,1.0583465315
C, -1.0803720211,3.3439141236,0.5114749144
C, 0.2863281724,3.5098507184,0.1834606609
C, 0.8584418676,4.7735754859,0.3947961913
H, 0.5719653739,6.7854208904,1.0724984468
H, -1.8097792186,6.4376780188,1.6877638825
H, -2.8527546337,4.2255891774,1.3621208263
H, 1.8888996221,4.9372849973,0.1038807289
N, -1.6247309758,2.0561794612,0.295330567
N, 0.9483054035,2.4306853739,-0.3946845551
C, -2.8803449016,1.7343464653,0.099177935
H, -3.5902665964,2.5550140629,0.0762639541
C, 2.2033565724,2.1835461191,-0.1345944887
H, 2.7362111117,2.7754801005,0.6178262233
C, -3.383119317,0.4236138564,-0.1153474954
C, -4.7689755048,0.2950043968,-0.3958972733
C, -2.564056439,-0.7458546873,-0.0769796174
C, -5.3661382302,-0.9232193458,-0.6510117344
H, -5.3567151953,1.2043977739,-0.4072442058
C, -3.1621029248,-1.9826186924,-0.3531051931
C, -4.5165327881,-2.0529344852,-0.6281621498
H, -2.5660940566,-2.8834910821,-0.3614723543
H, -4.9316591292,-3.0320007471,-0.8375999574
C, 2.9380545935,1.1276778698,-0.7525125547
C, 4.2489098927,0.8397448162,-0.2969414849
C, 2.3681877708,0.3148805753,-1.7680846852
C, 4.9926498855,-0.2107497308,-0.7939017
H, 4.6429327496,1.4640428443,0.495303147
C, 3.1260904201,-0.7254959049,-2.3030241851
C, 4.3913403487,-0.9843359332,-1.8134499548

H, 2.6827073366,-1.3510555513,-3.0674277032
 H, 4.9267152161,-1.8331900621,-2.2189927446
 O, -1.2787716128,-0.5710553055,0.2180898556
 O, 1.1166591653,0.506902535,-2.2226279313
 H, 0.7369272732,1.2628393572,-1.7198584986
 C, 6.3952299795,-0.5744545257,-0.2829843294
 C, 6.4388361194,-2.0764772274,0.0849492074
 H, 7.3884948175,-2.3092457215,0.5771444383
 H, 5.6076773692,-2.3538658216,0.7350900139
 H, 6.3646266506,-2.7125206035,-0.7999353802
 C, 7.4308403987,-0.2817465174,-1.39331748
 H, 8.4349561334,-0.5647674779,-1.0618410736
 H, 7.2096632616,-0.8461417559,-2.3029767401
 H, 7.4438682336,0.7813365505,-1.6526485678
 C, 6.7772655105,0.238659878,0.9670402476
 H, 6.8142577906,1.3140656757,0.7666560464
 H, 6.0765064842,0.0611774499,1.7873613647
 H, 7.7709756108,-0.0623810002,1.3085767442
 C, -6.863216772,-1.0912826191,-0.95430757
 C, -7.499267474,-2.0149500934,0.1104670088
 H, -7.3966773677,-1.5884285398,1.1117591369
 H, -8.5651264078,-2.1492464851,-0.0947395269
 H, -7.0383198433,-3.0053901276,0.1203069707
 C, -7.6103163187,0.2541202722,-0.9356824485
 H, -7.5498241026,0.739763345,0.0424277379
 H, -7.2264181037,0.9453130788,-1.691519243
 H, -8.6680737419,0.087896424,-1.1529163989
 C, -7.0354057193,-1.723705521,-2.3549920276
 H, -6.5633590366,-2.706650168,-2.4206669398
 H, -8.0974906498,-1.8520069833,-2.5821626848
 H, -6.5964211962,-1.0885951591,-3.1290380233
 H, -0.9503262637,1.2881455627,0.242578611
 C, 2.2411416153,-3.1091577881,0.6509622557
 O, 3.3891409276,-3.3547274532,0.3294713634
 O, 1.2025924571,-3.7657288128,0.8030823705

Zero-point correction=	0.632871 (Hartree/Particle)
Thermal correction to Energy=	0.672396
Thermal correction to Enthalpy=	0.673340
Thermal correction to Gibbs Free Energy=	0.558575
Sum of electronic and zero-point Energies=	-2187.334938
Sum of electronic and thermal Energies=	-2187.295413
Sum of electronic and thermal Enthalpies=	-2187.294469
Sum of electronic and thermal Free Energies=	-2187.409234

K

C, -1.0083166534,2.1425372914,1.3814828434
C, -2.2770916606,2.9660914505,1.1211302815
H, -0.4371207785,1.9358222367,0.47924495
H, -2.5786037032,2.9328430869,0.0735734217
H, -2.2037455698,3.9976469376,1.4605504794
O, -1.5454617395,0.8907902205,1.8616603744
C, -0.085884548,2.6839469667,2.4653430427
H, 0.7163809156,1.976312535,2.6517313736
H, -0.6268477345,2.9124448947,3.3827180183
Cl, 0.6897720566,4.2302135649,1.9129221852
C, -0.2105731979,-5.6488403885,0.4476172536
C, 1.1231235792,-5.5527970423,0.8347777448
C, 1.785583118,-4.3329459561,0.7363794076
C, 1.1317607785,-3.1942161456,0.2514655431
C, -0.2336831295,-3.2831898176,-0.1107578071
C, -0.8792589801,-4.5223375744,-0.0218032897
H, -0.731234486,-6.5974797379,0.5075953673
H, 1.646957223,-6.4212356232,1.2168172744
H, 2.8116932848,-4.245032781,1.0744478192
H, -1.9061609874,-4.6038449756,-0.3586219822
N, 1.7585351457,-1.9392037171,0.1921254996
N, -0.8667228682,-2.1445526232,-0.6336196263
C, 2.9809124698,-1.8138527615,-0.1949538761
H, 3.5513338394,-2.6756685496,-0.5616024031
C, -2.0913589161,-1.870296456,-0.3399606542
H, -2.6472051182,-2.4660599409,0.3923276436
C, 3.6619692092,-0.53539687,-0.1833490999
C, 4.9956099208,-0.4485999829,-0.6312513855
C, 3.0083541182,0.6349329013,0.2713112312
C, 5.7052410821,0.744051838,-0.6412001796
H, 5.4608419302,-1.3645428763,-0.9754274704
C, 3.7119921402,1.8432280328,0.2687190692
C, 5.0222140401,1.8869029024,-0.1759329558
H, 3.208057509,2.7366607125,0.6176027321
H, 5.5306027676,2.8443191343,-0.1614430124
C, -2.7978906752,-0.7580534225,-0.9420858358
C, -4.1394583889,-0.5143017831,-0.5860270663
C, -2.1624440068,0.0941047339,-1.8780591247
C, -4.8792695117,0.5316121431,-1.1214264873
H, -4.5804678915,-1.1727797169,0.1514372001
C, -2.903285152,1.1417855612,-2.4389079321
C, -4.2235074241,1.3449436391,-2.068772559
H, -2.4185193518,1.7813487332,-3.1671417231
H, -4.7599328236,2.166573815,-2.5306600477

O, 1.7356712282,0.6182904748,0.7065390179
 H, 1.4067961964,-0.3198027051,0.6182609212
 O, -0.8784314891,-0.0572716456,-2.2329951268
 H, -0.5302004574,-0.8481882055,-1.7431406997
 C, -6.336328766,0.8221793389,-0.7231394229
 C, -7.2482238668,0.6743044023,-1.9625990654
 H, -8.2882922282,0.889139049,-1.6984383179
 H, -6.9598178646,1.3603789559,-2.7631089929
 H, -7.2019057674,-0.3427123348,-2.361734834
 C, -6.8367561482,-0.1396692873,0.3701417932
 H, -7.8658370523,0.1145832192,0.6377345583
 H, -6.8350923957,-1.1789873023,0.0289774455
 H, -6.2292032214,-0.0718569958,1.2761806954
 C, -6.4435107615,2.2644770451,-0.1745188669
 H, -5.8008679273,2.3958904665,0.6993038244
 H, -6.1549653201,3.0066571463,-0.9234442418
 H, -7.4745175044,2.4802506846,0.1220285908
 C, 7.1602181964,0.8602820005,-1.126479682
 C, 8.049621789,1.380516692,0.0265546556
 H, 8.027595479,0.6931826108,0.8766335458
 H, 9.0874416113,1.4772034788,-0.306844208
 H, 7.7227995555,2.3606743636,0.3819517039
 C, 7.7259246272,-0.4921913673,-1.5960370675
 H, 7.7318172048,-1.2328444802,-0.7914122686
 H, 7.1580685117,-0.900734144,-2.4365811707
 H, 8.758714712,-0.3621539686,-1.9297517754
 C, 7.2309689639,1.8487630907,-2.3135728837
 H, 6.878517466,2.8445936665,-2.0347798614
 H, 8.2622221085,1.9481506385,-2.6660317117
 H, 6.6177991283,1.4993527755,-3.1486093838
 C, -2.8503494867,1.0438608341,2.2137982147
 O, -3.2780113233,2.2915145278,1.9071762984
 O, -3.51605203,0.1971843857,2.7203190779

Zero-point correction=	0.632564 (Hartree/Particle)
Thermal correction to Energy=	0.672163
Thermal correction to Enthalpy=	0.673107
Thermal correction to Gibbs Free Energy=	0.555887
Sum of electronic and zero-point Energies=	-2187.394110
Sum of electronic and thermal Energies=	-2187.354511
Sum of electronic and thermal Enthalpies=	-2187.353567
Sum of electronic and thermal Free Energies=	-2187.470787

K'

C, 0.4407331813,-1.4079307546,2.3824447417
 C, 0.8777466373,-2.4768310033,1.378694638

H, -0.3431399512,-0.777665948,1.9698872684
H, 0.4913317366,-3.4701841322,1.5991053733
H, 0.6239956428,-2.1848578454,0.3602027959
O, 1.6450823843,-0.619409311,2.5283191688
C, 0.0765642013,-1.9233357341,3.7697928471
H, -0.0241233002,-1.0957322341,4.4678380649
H, 0.8156600078,-2.6322944966,4.1415273667
Cl, -1.5160227133,-2.7875931009,3.7349038008
C, 0.2634034861,5.5642167696,1.1686262523
C, -1.0904256217,5.3940252541,1.449724737
C, -1.7304366574,4.2105052063,1.0972434801
C, -1.0290746146,3.1944080522,0.444252337
C, 0.3482074515,3.3526638311,0.1661214819
C, 0.9736693928,4.5499618599,0.5351778264
H, 0.7652212352,6.4865572296,1.4361961863
H, -1.6476647535,6.1748370571,1.9532759347
H, -2.7709690953,4.063999783,1.3605448457
H, 2.0167139384,4.6934203833,0.2790240546
N, -1.6321905677,1.9755401432,0.089100005
N, 1.001737546,2.3387910351,-0.5452066966
C, -2.9243934037,1.75529996,-0.1390913696
H, -3.5837193292,2.6186209211,-0.123809629
C, 2.2038212698,1.9740704144,-0.2382898318
H, 2.7009366507,2.3769215643,0.6511169688
C, -3.4507104475,0.4920779089,-0.4094561932
C, -4.8483676916,0.3609320832,-0.6869097841
C, -2.579945211,-0.681955063,-0.4051169733
C, -5.4341564625,-0.8461079384,-0.9569563671
H, -5.4390977218,1.2698950278,-0.6758697607
C, -3.2337416558,-1.9311138534,-0.6916235715
C, -4.5725158262,-1.9950618303,-0.9512195335
H, -2.6166407167,-2.8219014455,-0.6999035094
H, -5.0034581313,-2.9679865296,-1.1637361584
C, 2.9538136486,1.0215754112,-1.0208771754
C, 4.2392526964,0.6325342974,-0.5852395313
C, 2.431807823,0.4747639857,-2.2208544956
C, 5.0227661672,-0.2715277698,-1.2843212728
H, 4.5932962774,1.0532079334,0.3468314787
C, 3.2203032495,-0.4294672169,-2.9407649676
C, 4.4744558018,-0.7876009521,-2.4777814509
H, 2.8192086172,-0.8435397809,-3.8579289729
H, 5.0458887559,-1.5009478871,-3.0610889334
O, -1.3410628264,-0.603283617,-0.1624316775
O, 1.2182183368,0.7914342836,-2.69254468

H, 0.8018478353,1.4131449891,-2.048849218
 C, 6.4027463873,-0.7442696053,-0.7979259808
 C, 6.8489117404,-0.0080853634,0.4786354294
 H, 7.8371518071,-0.367366665,0.7786993102
 H, 6.9273246534,1.0712499811,0.3158506266
 H, 6.1623559701,-0.190107715,1.3078925332
 C, 6.3304246478,-2.2565324061,-0.4795966968
 H, 7.3033582798,-2.617982574,-0.1315382922
 H, 5.5924963155,-2.4474773944,0.3029188516
 H, 6.0531599484,-2.8424885012,-1.3600704495
 C, 7.4603854122,-0.4942442497,-1.896772402
 H, 7.2295393692,-1.0300130738,-2.8208249307
 H, 7.5309487842,0.5706815235,-2.13608822
 H, 8.4445165372,-0.8315689803,-1.5574972862
 C, -6.9292667645,-1.0263716535,-1.2572152788
 C, -7.5578526814,-1.9693664092,-0.2043987179
 H, -7.4627937195,-1.5485242674,0.8002224977
 H, -8.6218972226,-2.1180512337,-0.4130331441
 H, -7.0813160111,-2.9525609691,-0.2003142912
 C, -7.693660037,0.3088637922,-1.2205198816
 H, -7.6359788929,0.7822469719,-0.2363677761
 H, -7.3151094065,1.0143101457,-1.9654495014
 H, -8.7501208661,0.1337571516,-1.4402899028
 C, -7.10373032,-1.6424886308,-2.665255377
 H, -6.6123123588,-2.6146651546,-2.748422609
 H, -8.1652058435,-1.7877096312,-2.8886668231
 H, -6.6799722027,-0.9880140725,-3.4316893826
 C, 2.7196671618,-1.3521235364,2.1184440214
 O, 3.8538473925,-1.0167205731,2.266116166
 O, 2.3146854803,-2.4981157463,1.5347125052
 H, -1.0571670228,1.1202577094,-0.0177823077

Zero-point correction=	0.632781 (Hartree/Particle)
Thermal correction to Energy=	0.672557
Thermal correction to Enthalpy=	0.673501
Thermal correction to Gibbs Free Energy=	0.554401
Sum of electronic and zero-point Energies=	-2187.389105
Sum of electronic and thermal Energies=	-2187.349330
Sum of electronic and thermal Enthalpies=	-2187.348386
Sum of electronic and thermal Free Energies=	-2187.467486

L

C, -0.8043206538,2.4187099607,-1.063535273
 C, -0.0963211915,1.2342758567,-1.7182462109
 H, -0.0582977471,2.9747462117,-0.4775862826
 H, 0.7735096951,1.5565258002,-2.2970884481

H, -0.7891576882,0.6745518355,-2.3554168039
O, -1.855051599,1.9631789396,-0.2348726274
C, -1.455410722,3.3633913075,-2.0663675352
H, -2.0011121724,4.1396730872,-1.5371797091
H, -2.1353987181,2.841016718,-2.7349487802
Cl, -0.2140976279,4.2053592436,-3.100131487
C, -3.3079484312,0.2411816293,5.1845704493
C, -1.9209010451,0.1367225551,5.2154399674
C, -1.2155410282,-0.1015150715,4.0392579377
C, -1.8808095915,-0.232316032,2.8139117414
C, -3.2875060159,-0.1239296567,2.7905090006
C, -3.9859666721,0.1095891124,3.9743861941
H, -3.8646297305,0.4319388176,6.0944772048
H, -1.3842216265,0.2499205971,6.1502302776
H, -0.132856749,-0.1539085639,4.0500029035
H, -5.0655910988,0.1977972241,3.9343175899
N, -1.1882411195,-0.4136720529,1.601619314
N, -3.9820805237,-0.2249522434,1.5543724246
C, -0.3735198255,-1.3958879169,1.4954591906
H, -0.279465834,-2.1148450703,2.3213206689
C, -4.4835200552,-1.3479525248,1.213192236
H, -4.3959054472,-2.2116461739,1.8831904428
C, 0.4230920064,-1.7423558014,0.3157610871
C, 0.9256447673,-3.0529380089,0.2437280294
C, 0.664697668,-0.8670936748,-0.764090251
C, 1.5987236194,-3.5486344328,-0.8707246735
H, 0.7461616236,-3.6959333659,1.0965867664
C, 1.317265084,-1.348454145,-1.8999443711
C, 1.7660165407,-2.6627658658,-1.9459701086
H, 1.4945713788,-0.6892194036,-2.74023527
H, 2.2751566586,-2.9943855322,-2.843590927
C, -5.2264080909,-1.6012913749,-0.026402764
C, -6.1160375003,-2.6861479539,-0.0276801215
C, -5.0899783645,-0.8476390436,-1.2089201247
C, -6.91159219,-3.020131146,-1.1263826802
H, -6.1867875437,-3.273162622,0.8821369403
C, -5.860492923,-1.1718589507,-2.3178439764
C, -6.7646393905,-2.2298105196,-2.2724288904
H, -5.729532695,-0.5873716693,-3.2203579762
H, -7.3467426887,-2.440435897,-3.1595386301
O, 0.2962352005,0.4199832396,-0.6048215181
H, -1.5352602655,1.1994681748,0.2817378169
O, -4.1342806885,0.1382912668,-1.3336906326
H, -4.4925810804,1.1377986789,0.6259417313

C, -7.8840555722,-4.2104301797,-1.0459750493
 C, -8.9095571855,-3.9613178303,0.0844146362
 H, -9.6104162186,-4.7987468463,0.1524757909
 H, -8.4244369002,-3.8551507913,1.0576901949
 H, -9.4847549673,-3.0508111519,-0.103293825
 C, -8.6581799249,-4.4156344349,-2.3606730663
 H, -9.3358668333,-5.266753507,-2.2569645627
 H, -9.2636743114,-3.542268892,-2.6173511326
 H, -7.9887209931,-4.6281565534,-3.1986294841
 C, -7.0922530153,-5.5041923644,-0.7457808805
 H, -6.3554552176,-5.7017123987,-1.5290178898
 H, -6.5606222505,-5.445245497,0.2069779489
 H, -7.7713703809,-6.3604392191,-0.6940234241
 C, 2.1435396973,-4.9850453556,-0.9584303317
 C, 3.6746603633,-4.9410040905,-1.1708521254
 H, 4.169678519,-4.4333955285,-0.3385990276
 H, 4.0787801587,-5.9555996683,-1.2396669792
 H, 3.9416636219,-4.4136859489,-2.0896567352
 C, 1.8595686795,-5.7949667372,0.3195815031
 H, 2.3246132134,-5.343107799,1.2001443066
 H, 0.7871409389,-5.8946172863,0.5090647337
 H, 2.269239265,-6.8027425248,0.212797689
 C, 1.4822652454,-5.7168382763,-2.1494003544
 H, 1.6874980202,-5.216528517,-3.098662682
 H, 1.8616068354,-6.740466846,-2.2247874144
 H, 0.3970998227,-5.7642284837,-2.0244926601
 C, -4.567437408,1.4819439142,-1.232860038
 O, -4.6277732393,2.1751090435,-2.2011184926
 O, -4.86536626,1.8228236579,-0.0022947198

Zero-point correction=	0.631960 (Hartree/Particle)
Thermal correction to Energy=	0.671568
Thermal correction to Enthalpy=	0.672513
Thermal correction to Gibbs Free Energy=	0.556283
Sum of electronic and zero-point Energies=	-2187.352582
Sum of electronic and thermal Energies=	-2187.312973
Sum of electronic and thermal Enthalpies=	-2187.312029
Sum of electronic and thermal Free Energies=	-2187.428259

M

C, 2.1898248394,2.6807510787,-1.3326099262
 C, 2.6975533389,1.3074307156,-1.7329695706
 H, 2.6520375218,3.0010161914,-0.3958682954
 H, 3.7684260401,1.3485299762,-1.9391632071
 H, 2.1534810604,0.9412265176,-2.608391948
 O, 0.7868206673,2.5326552991,-1.159755549

C, 2.4372206067,3.7413254731,-2.4052702847
H, 2.0195041815,4.6853346416,-2.0698370255
H, 2.007735529,3.4500642043,-3.3622909173
Cl, 4.2138169813,4.0305392052,-2.6837691358
C, -0.9545175206,1.337105239,5.0252873737
C, 0.3820728154,0.9538714354,5.2024881247
C, 1.1012338482,0.4691468529,4.1215801952
C, 0.479197906,0.348051706,2.8766211349
C, -0.8822876671,0.7008885964,2.6756484462
C, -1.5716317331,1.2279900527,3.7907838782
H, -1.5072445727,1.7500035994,5.8617333744
H, 0.8651428509,1.077428618,6.163560921
H, 2.1549387572,0.235897438,4.2263844381
H, -2.5893089909,1.5723194583,3.6573501399
N, 1.1749794681,-0.1311772904,1.7462972344
N, -1.3943567065,0.5256326675,1.4198182232
C, 2.107265582,-1.0475813821,1.7555292807
H, 2.2624628741,-1.5388425281,2.7109111723
C, -2.6460283326,0.1949620724,1.2598595206
H, -3.228494031,-0.0768144431,2.151860569
C, 2.9115102659,-1.4917184585,0.6568141054
C, 3.6021230653,-2.7153577532,0.8164410342
C, 3.0687095737,-0.7659093716,-0.5525249289
C, 4.3935351652,-3.2668587849,-0.1795405667
H, 3.4777155916,-3.2322560236,1.759565001
C, 3.8642486796,-1.3093158066,-1.5630150455
C, 4.4982110578,-2.5297773976,-1.3735465878
H, 3.9868071093,-0.787818519,-2.5018336266
H, 5.0994626723,-2.9146650207,-2.1887658085
C, -3.3554731821,0.04634247,0.0358485571
C, -4.6272090164,-0.5823967543,0.1120860635
C, -2.8213346211,0.4335642291,-1.2576713219
C, -5.3863107452,-0.9163864829,-0.9902535329
H, -4.9938570838,-0.8219737692,1.1068760434
C, -3.6070644228,0.029511219,-2.3859601097
C, -4.820241618,-0.6007141503,-2.2554789775
H, -3.2100574046,0.2789099525,-3.3636169803
H, -5.3620382878,-0.8503636883,-3.1600815001
O, 2.4472620681,0.4239310504,-0.622336046
H, 0.8381731991,0.2449930899,0.8535412797
O, -1.7438963972,1.0892158871,-1.425826265
H, -1.3517568368,2.2332704239,-0.6530946405
C, -6.7564327822,-1.6010060114,-0.8269151469
C, -7.6984799404,-0.6933784625,-0.0021863428

H, -8.6771275599,-1.1680079601,0.1266463141
 H, -7.2928066676,-0.4901409906,0.9918722071
 H, -7.8476955244,0.2672719615,-0.502445606
 C, -7.4336551805,-1.8805913874,-2.1818939251
 H, -8.4027301585,-2.3600043047,-2.0168163868
 H, -7.6124059774,-0.960397511,-2.7449255601
 H, -6.8356167731,-2.5515511436,-2.8048672471
 C, -6.5842940522,-2.9520534395,-0.0942507437
 H, -5.9279909358,-3.6190412491,-0.6601391328
 H, -6.1470715061,-2.8190686191,0.898386904
 H, -7.5516904484,-3.4500388397,0.0313086973
 C, 5.1312911334,-4.607746889,-0.032345202
 C, 6.6513960722,-4.3773844769,-0.1983785372
 H, 7.0307868342,-3.6948312954,0.5667961808
 H, 7.1894902717,-5.3250076868,-0.1053553
 H, 6.8957548164,-3.9538895485,-1.1754293459
 C, 4.8875820954,-5.2551175847,1.3427265805
 H, 5.2449934353,-4.6234935468,2.1609884169
 H, 3.8290367395,-5.473289098,1.5094226226
 H, 5.4288172727,-6.2024101147,1.4015320808
 C, 4.6361492572,-5.5854351181,-1.123397769
 H, 4.8208461381,-5.2021358933,-2.1297697802
 H, 5.1553964315,-6.5438888128,-1.0346024473
 H, 3.5629480302,-5.7696488377,-1.0269186227
 C, 0.1517245724,3.4486364274,-0.3241365712
 O, 0.7455609747,4.3815411505,0.1606905996
 O, -1.0948830838,3.1386432758,-0.1771231703

Zero-point correction=	0.631579 (Hartree/Particle)
Thermal correction to Energy=	0.670769
Thermal correction to Enthalpy=	0.671714
Thermal correction to Gibbs Free Energy=	0.557231
Sum of electronic and zero-point Energies=	-2187.349316
Sum of electronic and thermal Energies=	-2187.310126
Sum of electronic and thermal Enthalpies=	-2187.309181
Sum of electronic and thermal Free Energies=	-2187.423664

N

C, -1.6759571357,-3.1168672549,-0.7712178369
 C, -2.4413983458,-1.9591833159,-1.393432042
 H, -2.1133455283,-3.3832247261,0.1962917109
 H, -3.4976571381,-2.2041033414,-1.5176245934
 H, -1.9977797278,-1.6731631034,-2.3514836571
 O, -0.3529669126,-2.6614339628,-0.610856062
 C, -1.6701446904,-4.3566007282,-1.66556541
 H, -1.1201549903,-5.1440624973,-1.1608089563

H, -1.2368239539,-4.1425586792,-2.6409978667
Cl, -3.3530900854,-5.0091522014,-1.9684078619
C, 1.263317797,-0.5751575555,5.0801448578
C, -0.1012138746,-0.3034252435,5.2104697846
C, -0.8580633289,-0.0449304052,4.075553491
C, -0.2413591871,-0.0289302162,2.8244887086
C, 1.1463268606,-0.2495881146,2.6736702931
C, 1.8761695312,-0.5623644193,3.8353912539
H, 1.8475932232,-0.8235384776,5.958783652
H, -0.5789288359,-0.3435606911,6.1813476337
H, -1.9317235933,0.0847639629,4.1504462672
H, 2.9222421868,-0.8238773243,3.7413389721
N, -1.0027674993,0.1788335316,1.6430827851
N, 1.6607689259,-0.1731463552,1.3961363638
C, -1.9693159627,1.0501287686,1.5302248697
H, -2.0746266368,1.7307375004,2.3699186203
C, 2.8691689369,0.2300499955,1.206444796
H, 3.4462867579,0.6317228284,2.0514511643
C, -2.8802845301,1.2173785589,0.440649202
C, -3.6705963742,2.3902546094,0.4201541919
C, -3.0442407027,0.2527540332,-0.5889561346
C, -4.5785386964,2.6601808312,-0.590911742
H, -3.5314740064,3.0953038169,1.2300115925
C, -3.961212967,0.5099321789,-1.6118880014
C, -4.6947504267,1.6870529765,-1.6041538042
H, -4.0973845436,-0.202582645,-2.4134664825
H, -5.3882334647,1.8497815415,-2.4210117201
C, 3.5583778336,0.2964623075,-0.060296902
C, 4.7377272585,1.0730429787,-0.0891014653
C, 3.0873529586,-0.2933595715,-1.2717447215
C, 5.4470777732,1.3555919451,-1.2475688886
H, 5.0780535909,1.4800366889,0.8583461703
C, 3.7888760205,0.0240548667,-2.4498786118
C, 4.9219742988,0.8180528302,-2.4386563813
H, 3.4216268129,-0.4072661606,-3.3735717553
H, 5.4189621888,1.0047090398,-3.3823702146
O, -2.3041504014,-0.8512026889,-0.4752172575
H, -0.7495989952,-0.4059025162,0.8382302171
O, 2.0437683072,-1.0928751536,-1.3798079032
H, 1.8488730182,-1.7178609471,-0.5805503766
C, 6.7219865417,2.217265583,-1.1958007658
C, 7.762597054,1.5506351438,-0.2667074316
H, 8.6766396452,2.1514799568,-0.2210348129
H, 7.3844237212,1.4425516283,0.7527309914

H, 8.0269460189,0.5541965327,-0.6305306676
 C, 7.3640150837,2.3877411078,-2.5852527414
 H, 8.2665566701,2.9990752648,-2.4998499484
 H, 7.6556719374,1.4273772263,-3.0191194155
 H, 6.6912745274,2.8900284666,-3.2858813159
 C, 6.379281373,3.6235308589,-0.6517495643
 H, 5.6496302353,4.1224322938,-1.2955406585
 H, 5.9576488837,3.5758421723,0.3553420563
 H, 7.2778384042,4.2475228399,-0.6074794899
 C, -5.4288790752,3.9396475105,-0.6474336554
 C, -6.9284824654,3.5621295594,-0.6370246659
 H, -7.191299271,3.0223172571,0.2766473372
 H, -7.5447872864,4.464203269,-0.687797563
 H, -7.1972223331,2.9312971616,-1.4876860539
 C, -5.1557928822,4.8681582886,0.5494102645
 H, -5.393742908,4.3870709412,1.5024239308
 H, -4.1143463341,5.200689666,0.5790252488
 H, -5.7806595443,5.7608908324,0.4699086201
 C, -5.1015282205,4.7128622838,-1.9461028082
 H, -5.3167665496,4.1212236821,-2.8391074507
 H, -5.7008027541,5.6259789274,-2.002754559
 H, -4.0461248978,4.9959908253,-1.9782772589
 C, 0.494191378,-3.3887899897,0.3501953259
 O, -0.0251266106,-4.3230066575,0.9375135859
 O, 1.6286569129,-2.874296127,0.3800115166

Zero-point correction=	0.631761 (Hartree/Particle)
Thermal correction to Energy=	0.671089
Thermal correction to Enthalpy=	0.672033
Thermal correction to Gibbs Free Energy=	0.557082
Sum of electronic and zero-point Energies=	-2187.349606
Sum of electronic and thermal Energies=	-2187.310278
Sum of electronic and thermal Enthalpies=	-2187.309334
Sum of electronic and thermal Free Energies=	-2187.424285

G

C, 0.3500476649,-2.5959410442,2.6335929227
 C, 0.618917358,-1.1708982951,2.4388071614
 H, -0.4910411652,-3.013188142,2.0879708488
 H, -0.042861409,-0.6232586496,1.7738152527
 H, 1.6372690206,-0.8043951606,2.5658879791
 O, 0.0032276131,-1.6484998344,3.6569210233
 C, 1.4261470946,-3.5338913805,3.1003960641
 H, 1.0226349124,-4.3236816576,3.7332011067
 H, 2.2050416937,-2.9946230479,3.6359064996
 Cl, 2.2529058504,-4.402736179,1.7131044685

C, 0.2227872316,4.8866508438,1.9290909615
C, -1.0709151382,4.5378449211,2.316230114
C, -1.627647054,3.3353912297,1.8981974102
C, -0.9192473369,2.4290085437,1.0792301924
C, 0.4141882908,2.7823816666,0.7182700077
C, 0.9524362994,4.0062705325,1.1357496935
H, 0.6557959526,5.8338111095,2.2318482828
H, -1.6494999875,5.2057828127,2.9469676627
H, -2.6195871201,3.0530199138,2.2310163177
H, 1.94168447,4.2883582719,0.791052036
N, -1.4274062951,1.2029138679,0.7039949407
N, 1.1172390956,1.9117857348,-0.1285871157
C, -2.6718480115,1.1277946792,0.330169599
H, -3.2201129178,2.0726665723,0.1706303298
C, 2.3923209748,1.7722947083,-0.0572926831
H, 2.9835117486,2.27459163,0.719881418
C, -3.4557761159,-0.0318793688,0.0501954305
C, -4.7646491058,0.2080941472,-0.4500672978
C, -2.9952415358,-1.4073368465,0.2636912506
C, -5.6654389311,-0.7831380961,-0.7790341202
H, -5.0446779212,1.2503082509,-0.5728807027
C, -3.9713822453,-2.4214675858,-0.1080285727
C, -5.2143083124,-2.1248162726,-0.5921461298
H, -3.6552555799,-3.4515571868,0.0254898619
H, -5.8809351245,-2.9478646244,-0.8406844137
C, 3.1263712596,0.9343230287,-0.9906525899
C, 4.5229603821,0.8436653138,-0.899648727
C, 2.4509439294,0.1989779098,-2.002133317
C, 5.2938576254,0.0684262249,-1.7644784693
H, 5.0036904965,1.4143363036,-0.1104014941
C, 3.2158324158,-0.5797769145,-2.8768288516
C, 4.5978001419,-0.6400135262,-2.7579716357
H, 2.6953277086,-1.1434901603,-3.6419363867
H, 5.13784883,-1.2639214138,-3.458728989
O, -1.8806713279,-1.7230591812,0.7267432394
O, 1.1252885418,0.2228441859,-2.1468747953
H, 0.7451898964,0.7867255941,-1.4199308944
C, 6.824171329,0.0135517358,-1.6046065252
C, 7.1835302476,-0.5203764298,-0.198611373
H, 8.2705753158,-0.5700428096,-0.0716159432
H, 6.7843618503,0.1215312491,0.5901294163
H, 6.7740067935,-1.5226253516,-0.0483609151
C, 7.4856145445,-0.9081883345,-2.646114335
H, 8.5691818531,-0.9167296232,-2.4949209614

H, 7.1300744367,-1.9384025703,-2.5584747937	
H, 7.2961805748,-0.5675540221,-3.6679404423	
C, 7.418087709,1.4312132233,-1.7760990567	
H, 7.1890807233,1.8306521263,-2.7680746823	
H, 7.0151812803,2.1276261884,-1.036904178	
H, 8.5070689877,1.4099411258,-1.6582081453	
C, -7.0788702037,-0.5177658391,-1.318615511	
C, -8.132339251,-1.1360437841,-0.3681304847	
H, -8.0648002243,-0.6825978881,0.6247734644	
H, -9.147721228,-0.9770223926,-0.7515771505	
H, -7.9829963338,-2.2121226443,-0.2504418307	
C, -7.3847535966,0.9855382943,-1.4450769956	
H, -7.3197865708,1.4907840621,-0.4774942261	
H, -6.692858261,1.4801843146,-2.1321646731	
H, -8.3997993408,1.1286059929,-1.8306485487	
C, -7.2367146442,-1.1526981163,-2.7212864209	
H, -7.0606162322,-2.2308832985,-2.6945803765	
H, -8.2467498043,-0.9860998395,-3.1152439252	
H, -6.5177808186,-0.7180807973,-3.4212292762	
Zero-point correction=	0.599993 (Hartree/Particle)
Thermal correction to Energy=	0.637919
Thermal correction to Enthalpy=	0.638863
Thermal correction to Gibbs Free Energy=	0.523452
Sum of electronic and zero-point Energies=	-1998.198184
Sum of electronic and thermal Energies=	-1998.160259
Sum of electronic and thermal Enthalpies=	-1998.159314
Sum of electronic and thermal Free Energies=	-1998.274725

H⁻

C, 0.7452351725,2.9641728216,-1.1671549032
 C, 1.3297981722,1.5511604182,-1.2580272607
 H, 1.5799182547,3.6560006441,-1.0175744094
 H, 1.5184922445,1.2667067067,-2.2988727587
 H, 0.6413545361,0.8451066488,-0.7933059391
 O, -0.1327133546,3.1319080876,-0.0790866997
 C, -0.0144635817,3.3722264233,-2.4354662318
 H, -0.4672354791,4.3477812912,-2.2818141164
 H, -0.7720756803,2.6380245684,-2.6971445419
 Cl, 1.088897798,3.5704219114,-3.9069292512
 C, -0.9692483102,0.9855765373,5.1997256
 C, 0.4124804168,0.8460324675,5.3055705185
 C, 1.168806759,0.6316530933,4.1550261463
 C, 0.5667320851,0.5591154916,2.892426713
 C, -0.8456458844,0.6942513688,2.7770866615
 C, -1.5853541489,0.9107904127,3.9533414185

H, -1.5684836612,1.1752263215,6.0847833397
H, 0.9031632151,0.9277878687,6.2697149758
H, 2.24992781,0.5688417958,4.2176008286
H, -2.655641071,1.0595786294,3.866887504
N, 1.3156070984,0.4193173938,1.7230523751
N, -1.4178267001,0.6455859521,1.517114449
C, 2.2559178629,-0.4339693165,1.6439228355
H, 2.440454025,-1.1578262847,2.4548967712
C, -2.513998959,-0.0087753581,1.3328268224
H, -2.9216142527,-0.6121687597,2.1630158132
C, 3.1595318909,-0.5738192391,0.4934263788
C, 3.9840900694,-1.7135252979,0.4616518777
C, 3.2799779003,0.3722831812,-0.5469500774
C, 4.8960235309,-1.9720478223,-0.5593418239
H, 3.8787453813,-2.4136129823,1.2820624918
C, 4.1984093879,0.1279794564,-1.5716474912
C, 4.9851959001,-1.0154059607,-1.5822467292
H, 4.2882045728,0.8713820741,-2.3556077701
H, 5.6817471773,-1.1569027665,-2.4017266534
C, -3.2919592946,-0.0845453473,0.1241016035
C, -4.4433533647,-0.8997081346,0.1662037553
C, -2.9394519437,0.6152769011,-1.104569912
C, -5.3014588281,-1.0991031618,-0.9054073775
H, -4.6512421015,-1.3939513909,1.1136663911
C, -3.8446403959,0.3787913108,-2.200962091
C, -4.9564704149,-0.4257128546,-2.1033672125
H, -3.6091520349,0.8811107284,-3.1341227126
H, -5.5806774645,-0.5378309467,-2.9838616686
O, 2.5991884864,1.5486781178,-0.5523155899
O, -1.9336946045,1.3689283189,-1.2368840619
H, -0.81426213,2.4273255709,-0.1453964651
C, -6.5408530194,-2.0016908232,-0.7652654112
C, -7.4785668134,-1.4469208086,0.3334406354
H, -8.3627123454,-2.0849828012,0.4544732991
H, -6.9697659475,-1.3896864007,1.2985955468
H, -7.8153062775,-0.4382158108,0.078129919
C, -7.3495617819,-2.0883597835,-2.0731339921
H, -8.2204983284,-2.7364269423,-1.9297833398
H, -7.7127877868,-1.1062549989,-2.3883833909
H, -6.7524815703,-2.5059648129,-2.8885318748
C, -6.1127031034,-3.4372304771,-0.3792903357
H, -5.4628850573,-3.8638600572,-1.1485149612
H, -5.5590291379,-3.4484828234,0.5625617989
H, -6.9867213723,-4.0901597213,-0.2648784325

C, 5.7837695834,-3.2286696293,-0.5982104761	
C, 7.2729442877,-2.811627946,-0.5928394036	
H, 7.5147569146,-2.2486992636,0.3129483214	
H, 7.9190171699,-3.6953812528,-0.6298125331	
H, 7.5182471925,-2.1814783896,-1.4507892935	
C, 5.5437437255,-4.1550153653,0.6078038803	
H, 5.7672735378,-3.6553685165,1.554365812	
H, 4.5110412783,-4.5115687236,0.645927826	
H, 6.1946964975,-5.0312768669,0.533835687	
C, 5.4844255753,-4.0315401981,-1.8854698481	
H, 5.6776634993,-3.4407640794,-2.7837450277	
H, 6.1108909818,-4.9288494107,-1.9325474053	
H, 4.4369632103,-4.343315987,-1.9124455224	
Zero-point correction=	0.603027 (Hartree/Particle)
Thermal correction to Energy=	0.639733
Thermal correction to Enthalpy=	0.640677
Thermal correction to Gibbs Free Energy=	0.532508
Sum of electronic and zero-point Energies=	-1998.223276
Sum of electronic and thermal Energies=	-1998.186569
Sum of electronic and thermal Enthalpies=	-1998.185625
Sum of electronic and thermal Free Energies=	-1998.293794

F
 C, -0.6444033104,-2.2683904729,-1.8632256225
 C, -1.2750002659,-0.8946604002,-1.6116704897
 H, -1.4477610474,-3.009743953,-1.8536830295
 H, -1.4528042624,-0.3636775879,-2.5528031622
 H, -0.6208838443,-0.3093841423,-0.9658805383
 O, 0.2737608247,-2.6451719279,-0.8599086765
 C, 0.0938706357,-2.3463786943,-3.2049650655
 H, 0.5763426107,-3.3158846197,-3.2933404709
 H, 0.825187231,-1.5478959603,-3.2991923708
 Cl, -1.0405191942,-2.2275607542,-4.656368868
 C, 1.0132945878,-1.7241020082,4.8023213358
 C, -0.3720519398,-1.6571570469,4.9305468523
 C, -1.1390248181,-1.221692918,3.8518380016
 C, -0.5429599054,-0.854512701,2.6385287367
 C, 0.8725216105,-0.9123655109,2.5031389534
 C, 1.6228606023,-1.3572006293,3.6057723451
 H, 1.6211055491,-2.084435008,5.6262506236
 H, -0.8565207656,-1.9646281043,5.8512435136
 H, -2.2214777287,-1.2090355399,3.9222814757
 H, 2.6966851221,-1.4500906827,3.4920549011
 N, -1.3005986947,-0.4874915072,1.5240818625
 N, 1.4388775219,-0.5649112572,1.2879275151

C, -2.2626116517,0.338401971,1.6323193219
H, -2.4595315551,0.8618648182,2.5821920647
C, 2.5051368273,0.1592322513,1.2586122216
H, 2.8905870151,0.5814867631,2.2032279243
C, -3.1776789735,0.7039220965,0.542382659
C, -4.0379398833,1.793842108,0.7699152017
C, -3.2780872217,0.0135635182,-0.6846229638
C, -4.9687547843,2.2445463827,-0.1635179457
H, -3.9466124741,2.2941425127,1.7267644985
C, -4.2165868325,0.4492442031,-1.6238818876
C, -5.0397997779,1.5386370374,-1.3742987451
H, -4.290172519,-0.101948024,-2.5544387873
H, -5.7496839663,1.8364349182,-2.1385685229
C, 3.2736569253,0.5338722874,0.099477504
C, 4.3844776058,1.3745099227,0.3255210936
C, 2.9488165746,0.1072729669,-1.2541498561
C, 5.2244918758,1.848136109,-0.6719820296
H, 4.5740823224,1.6578316959,1.3593352819
C, 3.8331732783,0.6225309195,-2.2669711669
C, 4.9051888921,1.4397466385,-1.989917553
H, 3.6162601336,0.3271164194,-3.2888066925
H, 5.5171281428,1.7735064417,-2.8214166931
O, -2.5569752395,-1.1048385243,-0.963155883
O, 1.9787334971,-0.6470650954,-1.557220711
H, 0.943388491,-1.924884674,-0.778886511
C, 6.4140170635,2.7637593056,-0.3315534078
C, 7.3803589235,2.041251847,0.6365585991
H, 8.2316716076,2.683509702,0.8936838695
H, 6.8778763366,1.7615006974,1.5654986274
H, 7.7661164519,1.1249527092,0.1810253307
C, 7.2172810856,3.1655897868,-1.5832814681
H, 8.0506985191,3.8156846714,-1.2973276542
H, 7.6344061841,2.2920618342,-2.09220243
H, 6.5993673213,3.7121759507,-2.3011691788
C, 5.9080126509,4.0619113463,0.3409910421
H, 5.2302853064,4.6012084384,-0.3267116007
H, 5.3611389229,3.8458276619,1.2617776998
H, 6.7441687129,4.7259767504,0.5927400491
C, -5.8940538376,3.4490427605,0.0850655691
C, -7.3702947693,2.9964741918,0.0007182442
H, -7.5860552007,2.2344711091,0.7547032259
H, -8.0415045206,3.8454304757,0.1697146414
H, -7.6075643634,2.5724255051,-0.9777092549
C, -5.6688197722,4.0852562456,1.4687989786

H, -5.8691357382,3.3774736683,2.2777877503
H, -4.6459876706,4.4537321957,1.5833104409
H, -6.3446560448,4.9358939588,1.597132858
C, -5.6310654532,4.5314757875,-0.987591067
H, -5.8123672186,4.1528169448,-1.9960897306
H, -6.2869799489,5.3944924983,-0.8302166398
H, -4.5946787852,4.8766454187,-0.9438980985
C, -0.0147819587,-4.7793615302,0.6566952199
O, 0.9734969835,-4.5997855743,1.2371013329
O, -1.012676009,-5.0566495941,0.1282404122

Zero-point correction=	0.615415 (Hartree/Particle)
Thermal correction to Energy=	0.656452
Thermal correction to Enthalpy=	0.657396
Thermal correction to Gibbs Free Energy=	0.535622
Sum of electronic and zero-point Energies=	-2186.859931
Sum of electronic and thermal Energies=	-2186.818894
Sum of electronic and thermal Enthalpies=	-2186.817950
Sum of electronic and thermal Free Energies=	-2186.939724

J

C, -1.5468800046,-2.9373175729,-1.9689956991
C, -2.383408554,-1.6764869259,-2.117161379
H, -1.8914691055,-3.5166367629,-1.1088575248
H, -3.4050320705,-1.9315837831,-2.4184752013
H, -1.9307808953,-1.0166717571,-2.8664957832
O, -0.2054473233,-2.5384521787,-1.7930476158
C, -1.5808251951,-3.8261876691,-3.2129863007
H, -0.9584186869,-4.6944192096,-3.0236153317
H, -1.2492494354,-3.2882489643,-4.0995538551
Cl, -3.2567100601,-4.4825776648,-3.6134492629
C, 0.9844048176,-2.1979648742,4.7788465044
C, -0.3914080563,-2.0237145559,4.9012955522
C, -1.110264428,-1.4563598694,3.8518746183
C, -0.4737833216,-1.0571298948,2.6686598887
C, 0.9355407541,-1.1992802542,2.5544217621
C, 1.6356929312,-1.7881415775,3.6181839254
H, 1.5493838318,-2.6730731823,5.5740080082
H, -0.9104909999,-2.354763648,5.7946053019
H, -2.189629311,-1.3695787873,3.9124141333
H, 2.6989088295,-1.9629355645,3.5031038803
N, -1.1934416352,-0.6047955044,1.5664410463
N, 1.5509002681,-0.7703577662,1.380449388
C, -2.0649528835,0.3155565762,1.6671850742
H, -2.2066268032,0.8642202842,2.6136640427
C, 2.6808145273,-0.1771442916,1.4468611144

H, 3.1191719603,0.065821165,2.4295742924
C, -2.9257676725,0.7829540684,0.5731545969
C, -3.6590927437,1.9580609862,0.7918116246
C, -3.0444891913,0.131666406,-0.6816065145
C, -4.4793730843,2.5469011645,-0.1706497582
H, -3.5516170433,2.4199853347,1.7661559277
C, -3.8518094672,0.7199265298,-1.6649471881
C, -4.546038463,1.8965941388,-1.4090635917
H, -3.9447448067,0.253126659,-2.6359669865
H, -5.1579890261,2.3062798232,-2.2058145655
C, 3.4793185218,0.309914762,0.3273249555
C, 4.600435028,1.0890410462,0.6710532979
C, 3.1638259404,0.1314544489,-1.0556363633
C, 5.4171093799,1.7401269255,-0.2487615035
H, 4.811515087,1.1886175356,1.732345632
C, 3.9718469551,0.8265572612,-1.9819948622
C, 5.0551522,1.5982102631,-1.5990901569
H, 3.7166522578,0.7087469349,-3.0290574266
H, 5.6331035054,2.0855471459,-2.3754992564
O, -2.3915110192,-1.0258895222,-0.8452809136
O, 2.1763121602,-0.582980805,-1.544944575
H, 1.9258853256,-1.4929743347,-1.0837426388
C, 6.6259752403,2.5658359247,0.2262174297
C, 7.6035006528,1.6598015928,1.0104368467
H, 8.470520121,2.2331955019,1.3584407314
H, 7.1229178454,1.2143561779,1.8845486986
H, 7.963327513,0.8427393474,0.3791044404
C, 7.400068821,3.1922073124,-0.9488206647
H, 8.2514855954,3.7647755368,-0.5678147782
H, 7.789270987,2.4295004691,-1.6289942504
H, 6.7724972608,3.8755025989,-1.5277312101
C, 6.1508137961,3.713842095,1.1471408701
H, 5.4673408184,4.3794068742,0.612589999
H, 5.6226208825,3.3324328342,2.0241377627
H, 7.0025737883,4.3071588387,1.4994720509
C, -5.2783156041,3.8390164348,0.0746069432
C, -6.7874489268,3.5582269423,-0.1119354274
H, -7.1296967389,2.797345446,0.5949101192
H, -7.3726204145,4.4690446047,0.0555713028
H, -7.0090252768,3.1988821533,-1.1196171677
C, -5.0699205564,4.3932607302,1.4958871245
H, -5.392936399,3.6805516524,2.2597242719
H, -4.0223771697,4.6432224852,1.683948594
H, -5.6575799393,5.3069932146,1.6251737388

C, -4.8342936207,4.9252829841,-0.9324641726	
H, -4.9985917334,4.6091620205,-1.9653063172	
H, -5.3966801455,5.8515984037,-0.7722265375	
H, -3.7698476075,5.1470062165,-0.8185565829	
C, 0.6475729146,-3.4476772494,-1.0527699967	
O, 0.2073085286,-4.5688758449,-0.8269294657	
O, 1.7437613732,-2.9113738364,-0.7818536662	
Zero-point correction=	0.616360 (Hartree/Particle)
Thermal correction to Energy=	0.655546
Thermal correction to Enthalpy=	0.656490
Thermal correction to Gibbs Free Energy=	0.542337
Sum of electronic and zero-point Energies=	-2186.848392
Sum of electronic and thermal Energies=	-2186.809206
Sum of electronic and thermal Enthalpies=	-2186.808262
Sum of electronic and thermal Free Energies=	-2186.922415

2J

C, -0.4983251373,-2.074517757,-1.7894478655
 C, -1.6001384873,-1.0148560264,-1.9656379377
 H, -0.1556553887,-2.0041985011,-0.7548549121
 H, -2.5386463841,-1.4662913058,-2.2922522803
 H, -1.288595471,-0.2718511288,-2.6952473789
 O, 0.6470033959,-1.8527324126,-2.5861184405
 C, -0.9760131818,-3.5026754288,-2.0637738698
 H, -0.1525198698,-4.1970795431,-1.9196685801
 H, -1.3848577389,-3.5818319187,-3.0657687966
 Cl, -2.2992335138,-4.0564731125,-0.9003306592
 C, 1.00974716,0.1990252771,5.6026012403
 C, -0.3846035505,0.1855703678,5.5976112739
 C, -1.0752039749,0.2829857013,4.393905118
 C, -0.3920900897,0.4010895997,3.1741834231
 C, 1.0307578906,0.4102216836,3.1789127637
 C, 1.7057968994,0.3036732804,4.4033818566
 H, 1.5542262574,0.1054014132,6.5360329988
 H, -0.9334541948,0.0787787353,6.5271479643
 H, -2.1576220305,0.2253335203,4.3805767054
 H, 2.7894711945,0.2794828276,4.4146023385
 N, -1.0484168629,0.4361876812,1.9428906483
 N, 1.6401081111,0.4849189084,1.9290866685
 C, -2.065202403,1.1943252856,1.7885570851
 H, -2.3742061704,1.8673815428,2.6048306326
 C, 2.8944990779,0.6864367131,1.7115496637
 H, 3.6077272384,0.8980590832,2.520308101
 C, -2.8936240678,1.3368547974,0.5935473729
 C, -3.8964204436,2.3224554524,0.6697390131

C, -2.7434544241,0.6064032242,-0.6184244384
C, -4.7476421452,2.6463928348,-0.3806252945
H, -3.979702796,2.8512291345,1.6119055565
C, -3.5866275369,0.9438063737,-1.6936947115
C, -4.5541806406,1.9287100732,-1.5699464439
H, -3.4820432718,0.4299488733,-2.6376382471
H, -5.1730417464,2.1376421721,-2.4363387655
C, 3.4395975655,0.6182874393,0.3754694131
C, 4.8294198473,0.7399825148,0.1787703547
C, 2.5987034719,0.3756319197,-0.7503499284
C, 5.4238831142,0.6031159395,-1.0682168531
H, 5.4392615304,0.9334656033,1.0572945591
C, 3.1901751145,0.1962570628,-2.0094736408
C, 4.5631895678,0.3115115489,-2.1490486335
H, 2.5622350906,-0.0824243017,-2.8524110294
H, 4.9719228241,0.1526376868,-3.1389286427
O, -1.8211009245,-0.3552650327,-0.6848547859
O, 1.2731548676,0.3153116151,-0.6481807322
H, 1.0248031256,0.3542924374,0.3114577965
C, 6.9505185928,0.7409534552,-1.2223877234
C, 7.661408087,-0.3419306329,-0.3775706579
H, 8.7496003406,-0.2581487917,-0.477228546
H, 7.4140554497,-0.2510691746,0.682979464
H, 7.3636605175,-1.3422674851,-0.703009568
C, 7.4055391876,0.5775150009,-2.6844210951
H, 8.4918677577,0.694629457,-2.7477880463
H, 7.1538491267,-0.4100163215,-3.0793293399
H, 6.9496873933,1.328133487,-3.3354010038
C, 7.4007186414,2.1385748379,-0.7370420233
H, 6.9227323351,2.9251446147,-1.3273783726
H, 7.1389936471,2.3049783563,0.3108541442
H, 8.4866368031,2.2494890675,-0.8332657752
C, -5.8379977808,3.727150179,-0.2909601306
C, -7.2207359718,3.093547869,-0.5705517321
H, -7.4441172159,2.3125199599,0.161350269
H, -8.0096817017,3.8515599561,-0.5153768586
H, -7.2627125806,2.6396012467,-1.5633216779
C, -5.8900731969,4.3903976393,1.0976444441
H, -6.1088430737,3.6643896574,1.8856559439
H, -4.9486410543,4.8889077342,1.3441276394
H, -6.6798421697,5.1473284684,1.1155050038
C, -5.5639034317,4.831107657,-1.3385692526
H, -5.5482371433,4.4285642205,-2.3539927428
H, -6.3402871072,5.6027510649,-1.2959086685

H, -4.5969282777,5.3076734189,-1.1561027387	
C, 0.4548525868,-1.6109943116,-4.034949297	
O, 1.4983119814,-1.235779182,-4.5617233931	
O, -0.6966112909,-1.8117501029,-4.4525072649	
Zero-point correction=	0.618362 (Hartree/Particle)
Thermal correction to Energy=	0.657735
Thermal correction to Enthalpy=	0.658679
Thermal correction to Gibbs Free Energy=	0.543668
Sum of electronic and zero-point Energies=	-2186.844013
Sum of electronic and thermal Energies=	-2186.804640
Sum of electronic and thermal Enthalpies=	-2186.803696
Sum of electronic and thermal Free Energies=	-2186.918707

2K

C, 0.4495496841,2.0475428538,2.5342252191
 C, 0.3399577772,3.3089963733,1.6819463345
 H, 0.9126690794,1.2338768968,1.9768205073
 H, 1.0893259383,4.0634003196,1.9135904091
 H, 0.3665378946,3.06195961,0.6241298867
 O, -0.9476395939,1.7340924454,2.7877222723
 C, 1.0639365806,2.2371950357,3.9182628895
 H, 0.9553690216,1.3254018905,4.5007061568
 H, 0.6007083869,3.0709238813,4.4462574978
 Cl, 2.8427945602,2.6008925139,3.8477487248
 C, -0.5643749418,-3.8512876994,3.4724168288
 C, 0.8269839707,-3.7524147197,3.4603375547
 C, 1.4563977632,-2.8304216868,2.6320022985
 C, 0.7232635465,-1.9796477929,1.779774575
 C, -0.696571428,-2.1050152602,1.7827556576
 C, -1.3131271654,-3.0276974508,2.6373969683
 H, -1.062923382,-4.5428552521,4.1428692982
 H, 1.4230363294,-4.3775577627,4.1178966469
 H, 2.5344990269,-2.7209117576,2.6580655019
 H, -2.3964653482,-3.0677049484,2.6721759146
 N, 1.314683059,-1.0079344662,0.9983098592
 N, -1.4205543031,-1.256858756,0.9376714623
 C, 2.3616521606,-1.2998481582,0.2901604149
 H, 2.6697780987,-2.3581045232,0.2331524388
 C, -2.5334435947,-1.6004644355,0.3972457185
 H, -2.9451815069,-2.6119386057,0.5153608842
 C, 3.1820405912,-0.4231326288,-0.4883979812
 C, 4.2201099838,-1.0364754997,-1.2373497341
 C, 2.9948844651,1.0252502382,-0.5455197102
 C, 5.0954979921,-0.3506075432,-2.0557742319
 H, 4.3061658306,-2.1151073488,-1.1425180961

C, 3.9249170456,1.7080146784,-1.4267951695
C, 4.9061571688,1.0605410392,-2.1271371446
H, 3.8055362676,2.784804563,-1.4977589601
H, 5.5639884085,1.6531402785,-2.7591713786
C, -3.3061446938,-0.6767453534,-0.4147487073
C, -4.5375725771,-1.0863305094,-0.9593756584
C, -2.8417449315,0.6387520932,-0.6659738858
C, -5.3351699462,-0.251504976,-1.7322220572
H, -4.853160905,-2.101160552,-0.7456768562
C, -3.6414964956,1.4902018333,-1.4416518432
C, -4.849678816,1.0532727648,-1.9544165545
H, -3.284320023,2.4969331884,-1.6221794366
H, -5.4334843888,1.750198698,-2.5465352574
O, 2.1252551701,1.6573014163,0.0969922097
O, -1.67557687,1.0960847725,-0.207719335
H, -1.2294547734,0.3658329451,0.3032626481
C, -6.6831672251,-0.6845494258,-2.333923972
C, -7.046150128,-2.1354741174,-1.9693267448
H, -8.0090518036,-2.3985150453,-2.4175298944
H, -6.3022351213,-2.8447897038,-2.3424109202
H, -7.13507323,-2.2708546034,-0.8879736292
C, -7.8085962258,0.2365271023,-1.8081289443
H, -8.7748171887,-0.0533334916,-2.2355222901
H, -7.8824563913,0.1744469982,-0.7190804853
H, -7.6283222796,1.2822315431,-2.0679206052
C, -6.6201854625,-0.5812525784,-3.8757042058
H, -6.4034226966,0.4384718765,-4.2024433558
H, -5.8367678886,-1.2311830613,-4.2749288465
H, -7.5751626459,-0.8807623462,-4.3214041825
C, 6.220511813,-1.0164659815,-2.8622215202
C, 7.5906696619,-0.4377502884,-2.4345393852
H, 7.7737560293,-0.6312033246,-1.3739189358
H, 8.4055404448,-0.8895331623,-3.0133063033
H, 7.6322010925,0.6437223185,-2.5847679554
C, 6.2676385235,-2.5409840547,-2.6528510847
H, 6.4381273892,-2.7964677663,-1.6033927976
H, 5.3374060505,-3.0196946126,-2.9708417112
H, 7.0846006009,-2.9733193006,-3.2400667838
C, 6.0154551305,-0.7519958142,-4.3733582127
H, 6.00198633,0.3181881628,-4.5940309444
H, 6.8198570298,-1.2070481588,-4.9641780445
H, 5.0626577972,-1.1701964627,-4.7097286612
C, -1.7096304845,2.8375026934,2.5694799071
O, -2.8715147334,2.9179762657,2.8344590397

O, -0.9672203753,3.8316062366,2.0379917197	
Zero-point correction=	0.617223 (Hartree/Particle)
Thermal correction to Energy=	0.657073
Thermal correction to Enthalpy=	0.658018
Thermal correction to Gibbs Free Energy=	0.539134
Sum of electronic and zero-point Energies=	-2186.855652
Sum of electronic and thermal Energies=	-2186.815801
Sum of electronic and thermal Enthalpies=	-2186.814857
Sum of electronic and thermal Free Energies=	-2186.933741

TSA-C

C, -0.7829482204,5.091090567,0.1083599538
C, 0.5354244682,5.1302699886,-0.3383905015
C, 1.2486279357,3.946293828,-0.4962475129
C, 0.6648251372,2.7070124003,-0.2058753814
C, -0.6911811054,2.664811361,0.2029510753
C, -1.3900545115,3.8664137668,0.3707406775
H, -1.3408958989,6.0097888742,0.2482438197
H, 1.0076055402,6.078332989,-0.5684838449
H, 2.2620461867,3.9780610573,-0.8792546658
H, -2.4077702695,3.8306093757,0.741862697
N, 1.3264973346,1.4813834668,-0.3670252433
N, -1.2680139492,1.4179508042,0.4993872634
C, 2.5993358923,1.3527173355,-0.2185805015
H, 3.2355861313,2.1990216166,0.0662903312
C, -2.4251251715,1.1392810343,0.0291671912
H, -2.9344154801,1.8442345,-0.643043539
C, 3.2564516657,0.0731497535,-0.3860074907
C, 4.6591137166,-0.0136200973,-0.2809397123
C, 2.5050906045,-1.1050578156,-0.6208054117
C, 5.3470278249,-1.2119249858,-0.4103778798
H, 5.1967875899,0.9079487251,-0.0930296121
C, 3.1871874217,-2.3204334458,-0.744939927
C, 4.567037191,-2.3635565278,-0.6450250451
H, 2.6082371126,-3.2188307852,-0.9221934634
H, 5.0544723995,-3.3262164143,-0.7516177789
C, -3.1714598918,-0.0878275955,0.286662517
C, -4.4363116001,-0.1937829208,-0.3155924989
C, -2.7094425446,-1.1666016924,1.0826760171
C, -5.2707613284,-1.3021028089,-0.1705665283
H, -4.7640389108,0.6431080183,-0.9237553342
C, -3.5413999063,-2.2769577039,1.2399313584
C, -4.7871296549,-2.3472944069,0.6274019819
H, -3.1787567038,-3.091209854,1.8558269794
H, -5.3833370901,-3.236793438,0.7832558165

O, 1.1662531085,-1.0948746726,-0.714498249
 H, 0.8791616124,-0.1421019639,-0.6369188322
 O, -1.5168030704,-1.1888447634,1.7091509395
 H, -0.2405579355,-0.9368309316,1.5153677347
 C, -6.6405282041,-1.3390291332,-0.8719304454
 C, -6.4387890594,-1.2402709407,-2.401841075
 H, -7.4050408589,-1.2632868389,-2.9151635415
 H, -5.9335859495,-0.3140496564,-2.6855792787
 H, -5.8370331858,-2.0750801456,-2.7709639783
 C, -7.4113432159,-2.637680684,-0.5726628906
 H, -8.3753395352,-2.6179005944,-1.0877463447
 H, -6.8703599979,-3.5217840929,-0.9207346769
 H, -7.6109510002,-2.7554483415,0.495945338
 C, -7.5012761043,-0.1478154123,-0.391041673
 H, -7.6633052851,-0.1944504303,0.689189926
 H, -7.0299931347,0.8116334482,-0.6169350405
 H, -8.4785719341,-0.1618995107,-0.883238748
 C, 6.8777486793,-1.3254344535,-0.3088758971
 C, 7.4420096874,-1.8936930171,-1.6319551603
 H, 7.1976239777,-1.2391927652,-2.4730397072
 H, 8.5313393556,-1.9830780328,-1.5748357056
 H, 7.0386091503,-2.8847828121,-1.8525188938
 C, 7.5459918658,0.036623731,-0.0485749157
 H, 7.3475498431,0.7477674645,-0.8553200307
 H, 7.2095663892,0.4807662553,0.8923327293
 H, 8.6296184855,-0.0922191722,0.0172326305
 C, 7.2503898461,-2.2738408853,0.854433886
 H, 6.8408364751,-3.2761346381,0.7085753329
 H, 8.3377653468,-2.3676000071,0.9361882393
 H, 6.8687002517,-1.8925448623,1.8053715728
 C, -0.6561893504,0.0362631032,2.8225345638
 O, -1.2454422066,0.6262558222,3.6254665524
 O, 0.3965380379,-0.3205240366,2.2764258326

Zero-point correction=	0.545186 (Hartree/Particle)
Thermal correction to Energy=	0.578755
Thermal correction to Enthalpy=	0.579699
Thermal correction to Gibbs Free Energy=	0.478163
Sum of electronic and zero-point Energies=	-1534.576886
Sum of electronic and thermal Energies=	-1534.543317
Sum of electronic and thermal Enthalpies=	-1534.542373
Sum of electronic and thermal Free Energies=	-1534.643909

TSB-C

C, -0.7086606064,5.1408816889,-0.0090915881
 C, 0.63741293,5.1900302612,-0.3635506221

C, 1.3525809235,4.0128573885,-0.5543860618
C, 0.7415334069,2.7608159598,-0.3982417934
C, -0.630471992,2.7222183849,-0.066285763
C, -1.3355884851,3.908773437,0.1436537613
H, -1.2664582779,6.0541199179,0.1592085796
H, 1.1320601892,6.1455259741,-0.4939094358
H, 2.3896418138,4.0508167481,-0.8660196763
H, -2.3693154306,3.8642374097,0.4658829643
N, 1.4117699937,1.5573858537,-0.6442922935
N, -1.2376203196,1.4515324222,0.1185663428
C, 2.6102756434,1.3709302195,-0.202585419
H, 3.0932069673,2.1183084521,0.4377783071
C, -2.4538338206,1.2062309839,-0.2569340375
H, -2.9927173138,2.0143171942,-0.7521344913
C, 3.3792207523,0.1860078758,-0.4974931539
C, 4.6800318427,0.0580176143,0.0353312841
C, 2.8562570958,-0.852542119,-1.3071228192
C, 5.4832133637,-1.0447854183,-0.2074986159
H, 5.038197596,0.8692473183,0.6576245068
C, 3.6612744995,-1.9698611065,-1.5625231195
C, 4.9328744399,-2.0548755531,-1.0266005813
H, 3.2562997226,-2.7623610796,-2.1798848801
H, 5.5181098367,-2.9404882704,-1.2477566649
C, -3.1892828076,-0.0210021569,-0.0819183757
C, -4.5942994852,0.0422857072,-0.2395726698
C, -2.5740390018,-1.2709276468,0.1883097323
C, -5.4123446868,-1.0641577305,-0.071491447
H, -5.0273603032,1.0054587092,-0.4813667154
C, -3.3961786711,-2.391997218,0.3510690886
C, -4.771488057,-2.2834596124,0.2357201296
H, -2.918534796,-3.3398852073,0.5637915727
H, -5.3676802269,-3.1781826349,0.3755724909
O, 1.6300939691,-0.8093730241,-1.838323231
H, 1.1932608576,0.0181596617,-1.5253448906
O, -1.2413334298,-1.38691889,0.2033251262
H, -0.6325377841,0.6752314996,0.7816264476
C, -6.943360237,-1.0133735544,-0.2066970032
C, -7.3947843837,-1.9851004248,-1.3218233936
H, -8.4837686382,-1.9644746157,-1.4247024934
H, -6.9566965528,-1.7059583514,-2.283860307
H, -7.1019495575,-3.0155316083,-1.1081745975
C, -7.5892525881,-1.4333489291,1.1340865301
H, -8.6802237075,-1.4091486295,1.0543428475
H, -7.3002365104,-2.4458783155,1.4252376793

H, -7.2914988809,-0.7568498967,1.9396891302
 C, -7.4499728201,0.395455499,-0.5645421464
 H, -7.1939953811,1.1282688128,0.2059198968
 H, -7.0473663187,0.7432060189,-1.5201956226
 H, -8.5391927243,0.3815082748,-0.6538599226
 C, 6.9006258744,-1.2043204345,0.367080885
 C, 7.9170020141,-1.3245991663,-0.7920103894
 H, 7.9010557413,-0.4288213128,-1.4189201621
 H, 8.9311160429,-1.4481045332,-0.399480658
 H, 7.7017164384,-2.1835508274,-1.4319610095
 C, 7.3096436568,-0.0059201086,1.2426445169
 H, 7.3176012369,0.9288877841,0.6748894738
 H, 6.6421372604,0.117586038,2.0999097601
 H, 8.3193094012,-0.1625977547,1.6313927707
 C, 6.9639494479,-2.4804672505,1.2381271205
 H, 6.7265538627,-3.37770034,0.6617387023
 H, 7.9684945104,-2.6085889363,1.6530502767
 H, 6.2560030688,-2.421192376,2.0689302912
 C, -0.5283922127,-1.2741542486,1.5703412173
 O, -0.0786926544,-0.1067027111,1.6801190603
 O, -0.5135591272,-2.2643613658,2.2332952286

Zero-point correction=	0.547231 (Hartree/Particle)
Thermal correction to Energy=	0.580178
Thermal correction to Enthalpy=	0.581123
Thermal correction to Gibbs Free Energy=	0.480600
Sum of electronic and zero-point Energies=	-1534.621349
Sum of electronic and thermal Energies=	-1534.588401
Sum of electronic and thermal Enthalpies=	-1534.587457
Sum of electronic and thermal Free Energies=	-1534.687980

TSD-E

C, 1.00789342,-4.8754677856,-2.4332388625
 C, -0.4510304638,-4.7372706763,-2.3979752952
 H, 1.4782697061,-4.6911794586,-1.4600449445
 H, -1.006027108,-4.5231021553,-1.4991984144
 H, -1.007265443,-5.0106971555,-3.2836173566
 O, 1.1321921931,-3.8128478453,-3.3413665412
 C, 1.5583600626,-6.1461113464,-3.0592740776
 H, 2.6313384883,-6.0410903307,-3.2085776414
 H, 1.0705252682,-6.3520548422,-4.0096238922
 Cl, 1.2915887873,-7.5896899515,-1.9859992651
 C, -0.4927593456,-4.3239655739,3.3738371399
 C, 0.8276653579,-4.0131896203,3.6850219049
 C, 1.4976657003,-3.0292812529,2.9626133919
 C, 0.8678715586,-2.3447319805,1.9160690837

C, -0.4893116467,-2.6331364201,1.6261540242
C, -1.1443771618,-3.6339067128,2.3547073368
H, -1.0173742399,-5.0978593665,3.9222279142
H, 1.3366023023,-4.5303001225,4.4902677805
H, 2.5128740513,-2.7595432274,3.2300958958
H, -2.1648427949,-3.8897715314,2.0925368032
N, 1.4966398415,-1.3217689168,1.1921444308
N, -1.0957764626,-1.9643523791,0.5518991702
C, 2.7347076958,-1.4096128222,0.850035804
H, 3.3210658637,-2.3114306344,1.0686867361
C, -2.2879900179,-1.5235941416,0.6647529412
H, -2.8389427494,-1.6151780195,1.6120195802
C, 3.423830631,-0.3492839015,0.1463330835
C, 4.7832602351,-0.5007538021,-0.1760841317
C, 2.7491614277,0.8399775042,-0.2388323139
C, 5.5141298161,0.4712623361,-0.8519711133
H, 5.2645995755,-1.4255003457,0.1273203669
C, 3.4743543495,1.8237386481,-0.9165174729
C, 4.8176687964,1.6396831198,-1.2104902944
H, 2.95669623,2.7286937628,-1.2107768067
H, 5.3305045136,2.4328823422,-1.7389604148
C, -3.0355579965,-0.8562743132,-0.4043021561
C, -4.3997219052,-0.6027875741,-0.1709001341
C, -2.4876654405,-0.4227824575,-1.6220212166
C, -5.2262030445,0.0388203475,-1.0907287615
H, -4.803594726,-0.9327090054,0.7780442368
C, -3.2845173103,0.2339941434,-2.5485950044
C, -4.6310293322,0.4564937779,-2.290393713
H, -2.8288325235,0.5721285071,-3.4711248311
H, -5.2212183161,0.969096391,-3.0409125857
O, 1.4565379457,1.0524110747,0.0243225598
H, 1.1013005672,0.2393221207,0.4626329234
O, -1.1339167466,-0.5118967969,-1.9024001052
H, 0.9750803799,-2.6967489529,-2.8218317736
C, -6.7200352165,0.3050109842,-0.8351260756
C, -7.1845419499,-0.2327609744,0.5304829713
H, -8.249063325,-0.0228941506,0.6627294435
H, -7.0504008556,-1.3152216924,0.6088797693
H, -6.6511425791,0.2417422656,1.3587339028
C, -6.9832534495,1.8283939827,-0.8694463048
H, -8.0433058214,2.0341496891,-0.6930021633
H, -6.4034916948,2.3423850938,-0.0981603814
H, -6.715573761,2.2645086902,-1.8344666885
C, -7.5583955573,-0.3857961957,-1.9356331116

H, -7.3082035508,-0.0129907932,-2.9314989069
H, -7.3929760967,-1.4665423757,-1.931768097
H, -8.6246036733,-0.203889348,-1.7704387012
C, 7.0016565961,0.2430284245,-1.1769790246
C, 7.6211187179,1.4348327875,-1.9299482063
H, 7.5781466798,2.3551898143,-1.3409789157
H, 8.6736947301,1.2278855515,-2.1413483579
H, 7.1225475709,1.615675079,-2.8861305476
C, 7.7956730023,0.0402151198,0.1340431591
H, 7.7142480015,0.9198649023,0.7783467391
H, 7.4315579986,-0.8213488458,0.6991228794
H, 8.8554515357,-0.1273301754,-0.0826691371
C, 7.1512722309,-1.013973034,-2.0650385894
H, 6.598731014,-0.8969005901,-3.0011271009
H, 8.2042021182,-1.1875079442,-2.3091650075
H, 6.7739423925,-1.9096578602,-1.5657007326
C, -0.6045178536,-1.7136496664,-2.2539316464
O, -1.3510773128,-2.6825585282,-2.4694296056
O, 0.6603388693,-1.680756707,-2.3655474407

Zero-point correction=	0.624377 (Hartree/Particle)
Thermal correction to Energy=	0.664074
Thermal correction to Enthalpy=	0.665018
Thermal correction to Gibbs Free Energy=	0.547141
Sum of electronic and zero-point Energies=	-2187.282452
Sum of electronic and thermal Energies=	-2187.242756
Sum of electronic and thermal Enthalpies=	-2187.241811
Sum of electronic and thermal Free Energies=	-2187.359688

TSD'-E'

C, -0.026575335,-2.6857715494,-4.992121244
C, 1.3506070506,-2.4816444672,-5.0698773187
C, 2.0206302776,-1.9023179165,-3.9980962962
C, 1.322209637,-1.5587601829,-2.8406965599
C, -0.0677136488,-1.789323834,-2.7295746276
C, -0.7265068783,-2.3349304827,-3.843861407
H, -0.5608407601,-3.1017070097,-5.8386146286
H, 1.893525058,-2.7331360397,-5.9726895234
H, 3.0772745345,-1.6747559603,-4.077003865
H, -1.8016786566,-2.4599878016,-3.8071310187
N, 1.9772882683,-0.9373545988,-1.749555042
N, -0.6868268426,-1.4049398396,-1.5440212931
C, 3.2090399011,-1.1906549894,-1.3634780322
H, 3.688515777,-2.0317232793,-1.8563641706
C, -1.676485857,-2.0948121083,-1.1000442638
H, -1.9676939823,-3.0172449803,-1.6232070612

C, 3.9451031307,-0.4947518757,-0.3814874268
C, 5.2091031227,-1.0259379791,0.0079100383
C, 3.4711161698,0.7235652147,0.2039908523
C, 6.0006016696,-0.4247547883,0.9580213946
H, 5.5276597707,-1.9439224323,-0.4710961312
C, 4.2911439111,1.3372406491,1.1817784384
C, 5.4950563755,0.774288821,1.5346377972
H, 3.9383968728,2.2525241049,1.6395646659
H, 6.082534385,1.2801493283,2.2930339249
C, -2.5250749976,-1.8025527785,0.0415936635
C, -3.6542249704,-2.6393793327,0.1961787804
C, -2.3225905799,-0.7493645451,0.9645069663
C, -4.6098999867,-2.451030701,1.1824126381
H, -3.7636094768,-3.4495496864,-0.5147895773
C, -3.2907919396,-0.5401714985,1.9567521659
C, -4.3969849988,-1.3658641644,2.0535497554
H, -3.1661956282,0.2838920182,2.6438154163
H, -5.1132958421,-1.1603840403,2.8415384328
O, 2.3333620756,1.2231060194,-0.1920066778
O, -1.1723368641,-0.0550928918,0.9089651821
C, -5.8496496347,-3.3451452587,1.347264628
C, -5.8872042931,-4.485603883,0.3139690883
H, -6.7812007044,-5.0950273349,0.4715980032
H, -5.9257004156,-4.1044711647,-0.7103159431
H, -5.0188381544,-5.1443689021,0.4037378406
C, -5.8491206942,-3.976070875,2.7591800716
H, -6.73003192,-4.6118538988,2.8925750311
H, -4.9581714523,-4.5916714705,2.9104047161
H, -5.8659313452,-3.2159454476,3.5436025121
C, -7.1269222052,-2.4918437886,1.1692778379
H, -7.177778892,-1.6820625446,1.9006278867
H, -7.1591750801,-2.0426631685,0.1729676213
H, -8.0206503539,-3.1114684106,1.2941046878
C, 7.3619690661,-0.9752405269,1.409417216
C, 7.3214983408,-1.2698159551,2.9270807818
H, 6.5538273449,-2.0122173493,3.160897282
H, 8.2869232064,-1.659774211,3.26321359
H, 7.1062170374,-0.372475666,3.511967773
C, 7.7315788681,-2.2776335854,0.6776099766
H, 7.0024613383,-3.0707424206,0.8659098712
H, 7.8100189808,-2.1299332009,-0.4033058905
H, 8.7024915646,-2.6344078476,1.0305577494
C, 8.4625083525,0.0719684023,1.1193738496
H, 8.2782658882,1.0129409093,1.6431162076

H, 9.4379292517,-0.3020349631,1.4444883852
H, 8.5211196724,0.2905940538,0.0496638262
C, -1.1133976843,1.348682633,1.3018874917
O, -2.1403225052,2.0080392958,1.2298854882
O, 0.0563016551,1.6597745366,1.6089680226
H, 2.0883611171,2.1906868785,0.2909987809
C, 1.2160917407,4.4218894369,0.4946968079
C, 0.1962552781,3.9307556256,1.4204662014
O, 2.0301073153,3.358069814,0.9110367192
H, 0.9148230117,4.3753078729,-0.5587001612
H, -0.7903329312,3.599372667,1.1259301047
H, 0.3781987582,4.0780949881,2.4759490259
C, 1.8919202864,5.7480189499,0.7979148375
H, 2.7974760858,5.8421680948,0.2004132891
H, 2.1359863845,5.826956081,1.8554211812
Cl, 0.8235533744,7.1622105441,0.3850840429
H, 1.4421664435,-0.2480383315,-1.2116440889

Zero-point correction=	0.625726 (Hartree/Particle)
Thermal correction to Energy=	0.665385
Thermal correction to Enthalpy=	0.666329
Thermal correction to Gibbs Free Energy=	0.550155
Sum of electronic and zero-point Energies=	-2187.273178
Sum of electronic and thermal Energies=	-2187.233520
Sum of electronic and thermal Enthalpies=	-2187.232576
Sum of electronic and thermal Free Energies=	-2187.348750

TSE-F

C, 1.4135094048,0.0176273573,-4.5596666252
C, 1.8090095357,1.062539534,-3.5000369797
H, 0.871116848,0.5080837451,-5.3719855387
H, 2.0455755705,2.0378749502,-3.9136319482
H, 2.5989066331,0.721087836,-2.8331461475
O, 0.5155431323,-0.8785910073,-3.9344242021
C, 2.6136829886,-0.7307111499,-5.1275676063
H, 2.2870564052,-1.4715705698,-5.8527816578
H, 3.1985250149,-1.2060921413,-4.3413953415
Cl, 3.724782259,0.4126837757,-5.9966340247
C, 0.6448924342,4.2234412162,1.78296804
C, -0.6518432692,4.135709449,2.2805454614
C, -1.3795385049,2.961787492,2.1068436607
C, -0.8356137792,1.8633644948,1.4293380372
C, 0.4979684304,1.9388111089,0.9539144834
C, 1.2119739308,3.1311471247,1.1312694505
H, 1.2187848142,5.134951893,1.9063276175
H, -1.0944849735,4.9713147256,2.8104145904

H, -2.3718099735,2.8762314761,2.534791088
H, 2.2145464001,3.2013508005,0.7245152009
N, -1.5238645866,0.6503715383,1.2762718618
N, 1.0324563176,0.8514767535,0.2457015182
C, -2.7964670569,0.6173457084,1.0819072164
H, -3.3797647577,1.5396002538,0.9676857507
C, 2.1949882551,0.4187124585,0.5664324594
H, 2.7204477173,0.8580112549,1.427903459
C, -3.5303250086,-0.6265057684,0.9822482246
C, -4.9284310782,-0.5983449173,0.803770666
C, -2.8650188386,-1.8760632936,1.054876002
C, -5.6956221879,-1.7502612068,0.7058271917
H, -5.3974349052,0.3770358797,0.7476798863
C, -3.6308325897,-3.0454615122,0.9554456261
C, -5.0019672906,-2.9762493477,0.7883534541
H, -3.118166031,-3.9982706074,1.0105581078
H, -5.5530092288,-3.9073610583,0.7166030795
C, 2.941426739,-0.6503965168,-0.0856437573
C, 4.2155217561,-0.9321048916,0.4561733269
C, 2.4717747897,-1.4259256475,-1.1838922278
C, 5.0569103592,-1.9288888037,-0.017588611
H, 4.5292996911,-0.3208185834,1.2941494707
C, 3.3259452982,-2.4495919646,-1.6566216153
C, 4.5663147002,-2.6903996289,-1.0951406167
H, 2.9620711686,-3.0774131049,-2.4635281303
H, 5.1643984825,-3.4983789687,-1.503128216
O, -1.5428896581,-1.9821580471,1.2117700758
H, -1.1687960896,-1.0630913311,1.2357351118
O, 1.2963810863,-1.2543372334,-1.7592941286
H, 1.0016654961,-1.3439409309,-3.0850842874
C, 6.441314793,-2.2307599975,0.5796957566
C, 6.7997636478,-1.2737039051,1.730801582
H, 7.7915673237,-1.5199580306,2.1195169506
H, 6.8244679098,-0.231700494,1.3995745601
H, 6.0921608391,-1.3535386367,2.5604639767
C, 6.4613485971,-3.6756648642,1.1307849799
H, 7.4443680889,-3.9122226682,1.5501978728
H, 5.7146767234,-3.8006260491,1.919496702
H, 6.2470574753,-4.4098267475,0.3504482904
C, 7.5215092438,-2.0882066999,-0.5176639135
H, 7.3455872539,-2.7717070346,-1.3517985125
H, 7.5383426313,-1.0705644171,-0.9177195762
H, 8.5128321602,-2.3102860191,-0.1102645152
C, -7.2216424678,-1.7406257418,0.5143751635

C, -7.7906452294,-0.3114345022,0.4533884152
 H, -7.3752507783,0.2554113491,-0.3844530082
 H, -8.8747793505,-0.3521676201,0.3181577776
 H, -7.5946027508,0.2440392815,1.3748118062
 C, -7.5822999978,-2.4577204474,-0.8074211023
 H, -7.1250359402,-1.9515346932,-1.6618773368
 H, -7.2398592677,-3.4953233357,-0.8130617499
 H, -8.6668644394,-2.4646988606,-0.9549620858
 C, -7.8968163399,-2.4764314204,1.6951868416
 H, -7.6641721227,-1.9849689248,2.6437907126
 H, -8.9843691492,-2.4814191864,1.5711154796
 H, -7.5663967076,-3.5153090255,1.7683592273
 C, -0.095517757,0.2621094548,-2.3975200002
 O, 0.6149221839,1.2782537818,-2.6893161851
 O, -1.1074216336,-0.0620865093,-1.9620236955
 Zero-point correction= 0.627468 (Hartree/Particle)
 Thermal correction to Energy= 0.666684
 Thermal correction to Enthalpy= 0.667629
 Thermal correction to Gibbs Free Energy= 0.551773
 Sum of electronic and zero-point Energies= -2187.293770
 Sum of electronic and thermal Energies= -2187.254554
 Sum of electronic and thermal Enthalpies= -2187.253609
 Sum of electronic and thermal Free Energies= -2187.369465

TSG-H

C, -0.9162479236,-2.5346513009,3.7952889284
 C, -0.3913172829,-2.1081263096,2.4932777246
 H, -1.5188839727,-3.4433962551,3.7502015983
 H, -0.6947835165,-2.5495877282,1.5581804135
 H, 0.2547817044,-1.2411686485,2.4726556018
 O, -1.7053006168,-1.348074998,3.8636529599
 C, 0.0377188048,-2.5418017135,4.9724636034
 H, -0.5225739017,-2.6365784669,5.9002662755
 H, 0.6398736127,-1.6360437104,4.993033998
 Cl, 1.1700135724,-3.9522213545,4.8710020378
 C, 0.4863069947,3.9784141933,3.2921919981
 C, -0.88432127,3.8508095396,3.5139569807
 C, -1.5902934216,2.8066577586,2.9276259536
 C, -0.9490040372,1.8696072046,2.1033812116
 C, 0.4389783739,2.02134411,1.8510713853
 C, 1.1375451404,3.0682258589,2.4685829087
 H, 1.0478194923,4.7724909467,3.7704422823
 H, -1.4000023776,4.5517898874,4.1606226857
 H, -2.6458507019,2.6744750832,3.1342094063
 H, 2.207899106,3.1541622151,2.3208108122

N, -1.6282743567,0.7640980311,1.5904154304
N, 1.0393718421,1.0833438203,0.9965881734
C, -2.6834743047,0.9323194408,0.8796889082
H, -2.9863538254,1.9496897276,0.5894639018
C, 2.1083318314,1.3335719447,0.321928917
H, 2.587882902,2.3186759463,0.3458903742
C, -3.5250208514,-0.1200331287,0.3382672884
C, -4.3905119908,0.2522372748,-0.7117273046
C, -3.4943081151,-1.485697607,0.7749471666
C, -5.1917468672,-0.6464578132,-1.4028508609
H, -4.3972243617,1.3001076713,-0.98923263
C, -4.293899149,-2.4014441407,0.0364424224
C, -5.1067197597,-1.9978367625,-0.9995729147
H, -4.2601210548,-3.4393394595,0.34775754
H, -5.7028921766,-2.7483807104,-1.507982772
C, 2.7270963566,0.3372603186,-0.5318227517
C, 3.9342603286,0.6312213158,-1.1866079251
C, 2.1305372589,-0.9355296374,-0.7283431929
C, 4.5856131717,-0.2769708166,-2.0180395611
H, 4.3624756124,1.614737099,-1.0201188056
C, 2.7699547263,-1.8531101401,-1.5613125918
C, 3.9688359573,-1.5284779897,-2.1839784517
H, 2.307395676,-2.8211806807,-1.711995829
H, 4.4251088527,-2.2759278783,-2.819687115
O, -2.8297448478,-1.926939093,1.7988310756
H, -2.3536137753,-1.3932852241,3.0383830606
O, 0.9629508718,-1.2709226337,-0.1521554498
H, 0.6487570612,-0.4741671547,0.35575169
C, 5.9121582796,0.1048177562,-2.7002405208
C, 6.9767564067,0.4147749561,-1.6225042085
H, 7.9254590886,0.6938549449,-2.0914261996
H, 6.6693060841,1.240665819,-0.9763368356
H, 7.1541560477,-0.4573942548,-0.9874147795
C, 6.4514892624,-1.0264538955,-3.5948152922
H, 7.3905417439,-0.7116406162,-4.057584443
H, 6.6555487208,-1.9359818228,-3.0232450567
H, 5.7550189358,-1.2757829761,-4.4001046097
C, 5.7005253187,1.3552274414,-3.5846436307
H, 4.9524867517,1.1629445155,-4.3584659784
H, 5.3620811033,2.213777299,-2.9997386802
H, 6.6361226082,1.6371879412,-4.0775347627
C, -6.1252266704,-0.2433545431,-2.5548701538
C, -7.5811147983,-0.6281800341,-2.2014454636
H, -7.9132403173,-0.1077265226,-1.299019478

H, -8.2565310371,-0.3578476745,-3.0194212346	
H, -7.6858608729,-1.7012176553,-2.0249093835	
C, -6.0867060329,1.2694261472,-2.8370515456	
H, -6.3978207853,1.8528660009,-1.9660991404	
H, -5.0885101767,1.6022468,-3.1344709964	
H, -6.7712187283,1.5082130123,-3.6555981037	
C, -5.7022390104,-0.9840819923,-3.8453337603	
H, -5.7504941503,-2.0686854138,-3.7235631577	
H, -6.361552555,-0.7123136629,-4.6759318345	
H, -4.6772803886,-0.7248549209,-4.1238817086	
Zero-point correction=	0.610451 (Hartree/Particle)
Thermal correction to Energy=	0.647779
Thermal correction to Enthalpy=	0.648723
Thermal correction to Gibbs Free Energy=	0.536387
Sum of electronic and zero-point Energies=	-1998.659971
Sum of electronic and thermal Energies=	-1998.622644
Sum of electronic and thermal Enthalpies=	-1998.621699
Sum of electronic and thermal Free Energies=	-1998.734035

TSG'-H

C, 0.071777151,1.1379357659,-2.1721274832
 C, -0.3817399691,2.0302254797,-1.1000349468
 H, -0.7394046062,0.8722012194,-2.8709773086
 H, -1.368021025,2.4671496316,-1.0612018457
 H, 0.3703682786,2.4308314397,-0.4363619095
 O, 0.4377443828,0.137604074,-1.2932050629
 C, 1.2856416093,1.6109366919,-2.9657505318
 H, 1.6593966675,0.7866798111,-3.5714117383
 H, 2.0678079466,1.9671044772,-2.2987549518
 Cl, 0.8934636339,2.9828061593,-4.1120303629
 C, 0.7210270396,-5.2036871898,-1.4858793237
 C, -0.6166605539,-5.0125616038,-1.8216215926
 C, -1.2708027037,-3.8519657296,-1.4189405107
 C, -0.6020966289,-2.8870555414,-0.6655679544
 C, 0.7556433958,-3.0680649155,-0.3272497878
 C, 1.3995496139,-4.2377483637,-0.7492181536
 H, 1.2370425162,-6.1058255011,-1.7934074818
 H, -1.1474304799,-5.7539022835,-2.4067990312
 H, -2.295720647,-3.6758281744,-1.7238463105
 H, 2.429572089,-4.399155493,-0.4535142835
 N, -1.2349128527,-1.6845849392,-0.258596407
 N, 1.3813362977,-2.1168100439,0.4858685574
 C, -2.4939537014,-1.6199394453,0.117074527
 H, -3.0242596819,-2.5691520047,0.1456221602
 C, 2.540814448,-1.650149969,0.1758250915

H, 3.0323357344,-1.9458163377,-0.7574888702
C, -3.2239693332,-0.4675506577,0.4798537475
C, -4.618655234,-0.6116032593,0.7278529738
C, -2.5858824194,0.8231489837,0.6229493943
C, -5.4306294146,0.4559810498,1.0374685385
H, -5.0361430985,-1.6089804334,0.6485231744
C, -3.4542309923,1.9176301838,0.9285051284
C, -4.8009451492,1.7325981558,1.1191465824
H, -3.0061549839,2.8981098341,1.043958527
H, -5.4058809357,2.6003556811,1.3607791654
C, 3.2524342244,-0.7088429298,1.0120767154
C, 4.5335366831,-0.2684508845,0.6216403364
C, 2.6857189633,-0.2149242835,2.2122823004
C, 5.2783781507,0.6310178833,1.3708149874
H, 4.9290464034,-0.6666891324,-0.3051604017
C, 3.4270321632,0.6966281131,2.975091609
C, 4.6835266535,1.1006129923,2.561192921
H, 2.9880085613,1.0741564056,3.8907041328
H, 5.220156996,1.8073106104,3.1846524524
O, -1.3202618522,0.9437664196,0.5125927098
H, -0.6638291702,-0.8042324232,-0.3862345155
O, 1.4753287153,-0.5824463303,2.6458395083
H, 1.0895603165,-1.1936265834,1.9716789072
C, 6.6795168506,1.1173719013,0.9643322004
C, 7.6963158276,0.749456159,2.0699095842
H, 8.6994233254,1.089998849,1.7947126304
H, 7.4408391739,1.2100751378,3.0271147202
H, 7.7334405194,-0.3329783121,2.2200074113
C, 7.1557508259,0.4803016761,-0.3536912402
H, 8.1539300474,0.8508288835,-0.6017121174
H, 7.2179333865,-0.6089828116,-0.2789904045
H, 6.4953960568,0.7304058811,-1.1886355122
C, 6.6605564155,2.6523063857,0.7774488623
H, 5.9572207411,2.94023051,-0.0085473118
H, 6.3658410707,3.1690605152,1.6938646124
H, 7.6539311941,3.0151406093,0.4955022969
C, -6.9401219379,0.3346199496,1.2975380274
C, -7.7126704505,1.2055152273,0.2792861873
H, -7.5148782475,0.8758832977,-0.7443141505
H, -8.7900304747,1.135249443,0.4580061027
H, -7.4337806703,2.2595236688,0.3500189206
C, -7.4382957169,-1.1154323177,1.1626290983
H, -7.2708324961,-1.5116651483,0.1570549608
H, -6.9511931598,-1.7808219806,1.8808884649

H, -8.5134832828,-1.1538618381,1.3558112989	
C, -7.2573372219,0.8202925453,2.7313792366	
H, -6.9600497754,1.8605250134,2.8843312097	
H, -8.3313802393,0.7502147318,2.929189132	
H, -6.7335455437,0.2112323442,3.4729741072	
Zero-point correction=	0.612704 (Hartree/Particle)
Thermal correction to Energy=	0.649698
Thermal correction to Enthalpy=	0.650642
Thermal correction to Gibbs Free Energy=	0.540060
Sum of electronic and zero-point Energies=	-1998.665048
Sum of electronic and thermal Energies=	-1998.628054
Sum of electronic and thermal Enthalpies=	-1998.627110
Sum of electronic and thermal Free Energies=	-1998.737692

TSG'-H'

C, -0.4478632528,-2.2362121076,2.0865067322
 C, 0.43769575,-1.1930081135,2.634525389
 H, -0.999550942,-1.9288663857,1.1887440382
 H, -0.0285860455,-0.2390494385,2.7972823168
 H, 1.2104237285,-1.5027930312,3.3272459719
 O, -1.1500919796,-2.1584835005,3.291120803
 C, 0.0944236156,-3.6444357125,1.9238604444
 H, -0.7393368458,-4.3416288775,1.885368023
 H, 0.7532384684,-3.9119239593,2.7481031709
 Cl, 1.0401669102,-3.8945249046,0.3785185198
 C, -0.9516221905,5.7912085477,0.2744132183
 C, 0.4195534905,5.8202247993,0.0245903044
 C, 1.1535801324,4.6417882847,0.0683621737
 C, 0.5257101475,3.4223778298,0.3347158901
 C, -0.8710577335,3.3730159974,0.5739371608
 C, -1.5808806984,4.5860670803,0.5550834373
 H, -1.5255228132,6.7106082154,0.2729894171
 H, 0.9228477049,6.7585799951,-0.1741615467
 H, 2.2251399529,4.6852764069,-0.0799505243
 H, -2.635297957,4.570700323,0.802018664
 N, 1.2407435213,2.2063843785,0.4007180353
 N, -1.4605426056,2.1504961671,0.8934191939
 C, 2.4927185969,1.998954105,0.0298581783
 H, 2.9865068959,2.8228414669,-0.4743990679
 C, -2.6413552195,1.9023788434,0.4417512027
 H, -3.0900230815,2.5998691821,-0.2804893789
 C, 3.2465948812,0.8306018864,0.2486381801
 C, 4.5999091416,0.8022552115,-0.201335953
 C, 2.6984688813,-0.2973106014,0.9658360138
 C, 5.435351407,-0.2603983942,0.0439590104

H, 4.957480334,1.6679372393,-0.7467060252
C, 3.5844551378,-1.376045836,1.2322200447
C, 4.8811310743,-1.3477866357,0.7824794474
H, 3.2038804828,-2.2400874177,1.7602785222
H, 5.50713233,-2.2071345196,0.9966877393
C, -3.4867587606,0.7530408559,0.7134025856
C, -4.5815448487,0.5734146841,-0.1564003421
C, -3.2759187325,-0.2001212151,1.7477604624
C, -5.4398213555,-0.5195531372,-0.1035576267
H, -4.7313657001,1.3314627913,-0.9189170451
C, -4.1249693315,-1.3174477915,1.7940094956
C, -5.1686426136,-1.4712023094,0.8937128433
H, -3.9479591675,-2.0606918465,2.5631419226
H, -5.7896980482,-2.353175808,0.9863135937
O, 1.460981533,-0.2634236127,1.3132187117
O, -2.3162998295,-0.0190438494,2.6466443382
H, -1.9999276771,-0.9156897013,3.0529757279
C, -6.6055319037,-0.646892256,-1.1009370031
C, -6.0575659401,-0.656694841,-2.5466803306
H, -6.8774262001,-0.7477953593,-3.2661558272
H, -5.5118431703,0.2607387802,-2.7798479488
H, -5.3756193213,-1.4976290734,-2.6987889778
C, -7.4106971333,-1.9422097332,-0.887937589
H, -8.222453204,-1.9941579215,-1.6184555064
H, -6.7899676857,-2.8325347674,-1.0208043799
H, -7.8603533024,-1.9832833298,0.1079195421
C, -7.5678667267,0.5509428839,-0.9272931642
H, -7.975230363,0.5785722624,0.0869637029
H, -7.0643486725,1.5034757155,-1.109956312
H, -8.4047132584,0.4765077938,-1.6292206702
C, 6.8961465229,-0.3277434036,-0.4273285295
C, 7.0791006032,-1.545592696,-1.3632000815
H, 6.439599573,-1.4587398667,-2.2456301889
H, 8.1180790474,-1.6131979424,-1.6996422513
H, 6.8316032179,-2.4851946182,-0.8636178563
C, 7.3142045342,0.9371014632,-1.1977195097
H, 6.7108995451,1.0836051222,-2.0980804519
H, 7.2342100295,1.8348766563,-0.5782101877
H, 8.3570307171,0.8477522575,-1.512716942
C, 7.8293644247,-0.4770469345,0.7967229771
H, 7.6110256115,-1.3818036549,1.3690569536
H, 8.8732892342,-0.5345713187,0.4739491471
H, 7.7284086417,0.3777911352,1.4708869865
H, 0.7569147603,1.3997236118,0.8164329748

Zero-point correction=	0.614567 (Hartree/Particle)
Thermal correction to Energy=	0.651032
Thermal correction to Enthalpy=	0.651976
Thermal correction to Gibbs Free Energy=	0.543846
Sum of electronic and zero-point Energies=	-1998.692877
Sum of electronic and thermal Energies=	-1998.656412
Sum of electronic and thermal Enthalpies=	-1998.655468
Sum of electronic and thermal Free Energies=	-1998.763598

TSI-J

C, -1.0551994805,-2.884782318,-1.8019614449
 C, -1.4497532712,-1.419711428,-1.7319227758
 H, -1.8786450963,-3.4684732317,-2.2251565874
 H, -1.6369608019,-1.0312770991,-2.7376376722
 H, -0.6594717006,-0.8329123548,-1.2562538071
 O, -0.8152236863,-3.3616686116,-0.4666141576
 C, 0.2220897556,-3.1495492767,-2.592285676
 H, 0.4993931184,-4.1957666554,-2.49370538
 H, 1.0351497343,-2.5046234465,-2.2678778329
 Cl, -0.0243756394,-2.8455721483,-4.3708654602
 C, 0.8026969064,-1.7028465984,5.0913814625
 C, -0.5883266208,-1.7423057668,5.0449572523
 C, -1.2544423009,-1.3943164209,3.8739052047
 C, -0.5466885481,-1.0023045846,2.7318460044
 C, 0.8658942048,-0.9562585081,2.780179956
 C, 1.520830621,-1.3126284696,3.9659120792
 H, 1.3295748096,-1.9948642228,5.992319257
 H, -1.1559266064,-2.0644732977,5.9102215815
 H, -2.3336519335,-1.4686759299,3.815237115
 H, 2.6045923748,-1.3182101399,3.9857455591
 N, -1.2106880794,-0.701599194,1.5268881559
 N, 1.561477362,-0.579122873,1.6213380383
 C, -2.1254367156,0.1899978737,1.5491140717
 H, -2.3064164912,0.7613670212,2.4699790156
 C, 2.6109719037,0.1651443194,1.6753227144
 H, 2.9557439189,0.5908310817,2.6250007937
 C, -2.9850137854,0.5998322876,0.4313552481
 C, -3.6780332441,1.8154934172,0.5936956171
 C, -3.19698284,-0.1310251413,-0.7511471387
 C, -4.5310234622,2.3450988396,-0.3713075499
 H, -3.5186085376,2.3513780832,1.5211275472
 C, -4.0595479593,0.3742299724,-1.7215745041
 C, -4.7062760901,1.5890452801,-1.5404591432
 H, -4.2314581803,-0.2152468543,-2.6148158431
 H, -5.3691798842,1.94174087,-2.3219091368

C, 3.3795743224,0.4991021592,0.4924694584
 C, 4.5167882127,1.3229334045,0.6054053246
 C, 2.9987927569,0.0180670502,-0.7825178062
 C, 5.2914769254,1.6833166984,-0.4889081977
 H, 4.7759639439,1.6728189456,1.5974949747
 C, 3.7679371408,0.3753687822,-1.8939515905
 C, 4.8804672517,1.1859350942,-1.7425702072
 H, 3.4728911697,0.0060258453,-2.8688079462
 H, 5.4491214919,1.4381852032,-2.6305045596
 O, -2.6450094031,-1.3716283281,-0.9408912067
 H, -1.2832445517,-2.9101615521,0.5968544768
 O, 1.9243548614,-0.7727664348,-0.9512608239
 H, 1.5179564806,-0.9124746323,-0.0493138474
 C, 6.5392658831,2.5768420267,-0.384754434
 C, 7.7714721185,1.8082366917,-0.9156855366
 H, 8.6665639293,2.4347370192,-0.8535945503
 H, 7.9480664029,0.90252257,-0.329296696
 H, 7.646764799,1.5106801425,-1.9593533836
 C, 6.330893726,3.8553270256,-1.2297132326
 H, 7.2140131351,4.4988944583,-1.1706800801
 H, 6.1598852706,3.6220724788,-2.2833063024
 H, 5.4697135336,4.4248944956,-0.8699243385
 C, 6.8294704909,3.0021213975,1.0659350591
 H, 6.0073884078,3.5835927345,1.4925124377
 H, 7.0132516952,2.1396523157,1.7127217781
 H, 7.7242635089,3.6294288358,1.0928923504
 C, -5.2737205669,3.6809576601,-0.1962297358
 C, -6.7988350978,3.4326999341,-0.2591687315
 H, -7.1175876931,2.7559088224,0.5380954788
 H, -7.3419237075,4.3754088176,-0.1430149751
 H, -7.1001409993,2.9913931836,-1.2119516223
 C, -4.9516334128,4.3567258764,1.1490533246
 H, -5.2485004893,3.7358282062,1.9988037332
 H, -3.8867872821,4.5860161466,1.2451692252
 H, -5.4988852965,5.299763486,1.2250074936
 C, -4.863628103,4.6473427552,-1.331772882
 H, -5.1075923036,4.2440086265,-2.3172431912
 H, -5.3869522934,5.6021405045,-1.2244563363
 H, -3.7884237615,4.8441520326,-1.3079763971
 C, -1.8748607955,-4.413537104,0.2371601632
 O, -1.9845999213,-3.7253784677,1.2776256198
 O, -2.2214382643,-5.3860698818,-0.323570041

Zero-point correction=

0.626493 (Hartree/Particle)

Thermal correction to Energy=

0.666144

Thermal correction to Enthalpy=	0.667088
Thermal correction to Gibbs Free Energy=	0.550165
Sum of electronic and zero-point Energies=	-2187.319648
Sum of electronic and thermal Energies=	-2187.279997
Sum of electronic and thermal Enthalpies=	-2187.279053
Sum of electronic and thermal Free Energies=	-2187.395976

TSI'-J'

C, -0.9647113097,-2.7243829522,-0.7561163214
 C, -1.7931227294,-1.8890499311,-1.781842834
 H, -1.3810102752,-2.4678742148,0.2469492552
 H, -1.2163882311,-1.7912738014,-2.6962872532
 H, -2.784604301,-2.2911209093,-1.998885953
 O, 0.3570604444,-2.5006058169,-0.8350383951
 C, -1.2363086897,-4.2295560053,-0.9745202751
 H, -0.6169238413,-4.7983795968,-0.2880185975
 H, -1.0468227031,-4.5349686285,-2.0016862411
 Cl, -2.9877304698,-4.7694402841,-0.6213477536
 C, 1.2033017498,5.3090792267,-2.6061746127
 C, -0.1879835349,5.38209271,-2.5875952272
 C, -0.9272298511,4.2872671648,-2.1548738449
 C, -0.2819827698,3.1254331615,-1.7278262581
 C, 1.1258496094,3.031926954,-1.7521711651
 C, 1.849037211,4.1463774375,-2.2012142255
 H, 1.7874913751,6.1518930043,-2.9565369395
 H, -0.6971611088,6.2739056776,-2.9312774775
 H, -2.0101988772,4.3205312073,-2.1780648724
 H, 2.9287415459,4.072617955,-2.2525287754
 N, -1.0357399815,2.0296945197,-1.228225513
 N, 1.7460567255,1.8379666524,-1.3828517402
 C, -2.1176368302,2.1680547541,-0.4865399894
 H, -2.339120152,3.1885243239,-0.190917764
 C, 2.7179861148,1.8572307649,-0.5243979168
 H, 2.9595916991,2.7890583635,0.0015980432
 C, -2.9947703666,1.161758502,-0.0280433821
 C, -4.0287725268,1.5637909311,0.8664390908
 C, -2.907411547,-0.2065500912,-0.4283830922
 C, -4.9489736208,0.679150799,1.3818092713
 H, -4.0642080828,2.6112669032,1.138686245
 C, -3.84704855,-1.1114760119,0.0937685681
 C, -4.8217521189,-0.6703894766,0.9669334952
 H, -3.7993080632,-2.1594361264,-0.1639281972
 H, -5.5163161571,-1.4099594427,1.3482563316
 C, 3.5246729087,0.7167087411,-0.194826344
 C, 4.4470823481,0.8152320386,0.875355886

C, 3.4479453248,-0.4884957926,-0.937703331
 C, 5.2719522112,-0.2312584852,1.2416948895
 H, 4.4809868799,1.7555962258,1.4125093046
 C, 4.2802338915,-1.5565422189,-0.5748070056
 C, 5.1545982759,-1.422049437,0.4840380682
 H, 4.1825787506,-2.4836769002,-1.1233997887
 H, 5.7704187244,-2.2769226718,0.7402344358
 O, -1.9571818983,-0.5130687916,-1.3054982359
 O, 2.6472156327,-0.6343762688,-1.9938854665
 H, 2.0450548755,0.1352512879,-2.0404569041
 C, 6.2743428271,-0.1571282711,2.4048883733
 C, 5.9232509273,-1.2345587231,3.457275729
 H, 6.6341443944,-1.2007082469,4.2887692738
 H, 4.9194232981,-1.0736664061,3.8593829932
 H, 5.9539465367,-2.2410986258,3.0341664722
 C, 7.7035210691,-0.4092632099,1.8708211598
 H, 8.4292146474,-0.3701950231,2.6890859722
 H, 7.7918934388,-1.3887127654,1.3953259382
 H, 7.9823184418,0.3466752659,1.1315037421
 C, 6.2571614504,1.2159297815,3.100318706
 H, 6.5254551711,2.0233898277,2.4130404131
 H, 5.2772778823,1.4409200312,3.5307915837
 H, 6.9842183827,1.2239661677,3.9167577408
 C, -6.0661274033,1.0802383316,2.3573030931
 C, -5.8949424897,0.2974936739,3.6800191726
 H, -4.9337469079,0.5252929049,4.1483312054
 H, -6.6885460534,0.5667428424,4.3829357018
 H, -5.943390081,-0.7827354451,3.5251720062
 C, -6.0405156192,2.5847507953,2.679899979
 H, -5.1021660323,2.883944173,3.1555050517
 H, -6.1867630922,3.1967655681,1.7851727971
 H, -6.8492813591,2.8235068587,3.3748013868
 C, -7.4395437476,0.740864898,1.7326911753
 H, -7.5368638845,-0.3249335573,1.5138198738
 H, -8.2446892759,1.0111811866,2.4219064888
 H, -7.5925658825,1.2895407116,0.7993960157
 H, -0.7091962201,1.0812710507,-1.4215338677
 C, 1.3969103262,-3.2463608664,-2.5502042564
 O, 2.3292644215,-3.7284718051,-2.0269874498
 O, 0.6796433629,-2.9337129142,-3.4346337123

Zero-point correction=	0.629866 (Hartree/Particle)
Thermal correction to Energy=	0.669664
Thermal correction to Enthalpy=	0.670608
Thermal correction to Gibbs Free Energy=	0.554374

Sum of electronic and zero-point Energies=	-2187.321777
Sum of electronic and thermal Energies=	-2187.281980
Sum of electronic and thermal Enthalpies=	-2187.281036
Sum of electronic and thermal Free Energies=	-2187.397270

TSJ-K

C, -0.9136095526,1.8537169523,1.8989438068
 C, -0.1370857471,1.2988047015,0.7614639389
 H, -0.2756467283,1.8286871091,2.7929299172
 H, 0.7091302212,1.8951162615,0.4455901739
 H, -0.6462544074,0.7567198498,-0.0226148863
 O, -2.1345273497,1.1997459303,2.1116649549
 C, -1.2944721095,3.3253489666,1.6206134643
 H, -1.952499502,3.6594377179,2.4171484563
 H, -1.7894473236,3.439403023,0.6590081511
 Cl, 0.1493382734,4.424100577,1.6255154609
 C, -0.3226769784,-6.0272912616,-0.2064831672
 C, 0.9612300277,-5.9335250522,0.3199807431
 C, 1.5838363112,-4.6900346037,0.4042590708
 C, 0.9325343021,-3.5354981821,-0.0360651964
 C, -0.3697687728,-3.6274786766,-0.5719854753
 C, -0.9794787256,-4.8817382087,-0.651677547
 H, -0.8170457463,-6.989423471,-0.2740066275
 H, 1.4755809136,-6.8187566139,0.6749307471
 H, 2.5640085314,-4.5981481767,0.8585768466
 H, -1.9665907182,-4.9516716566,-1.0938828043
 N, 1.512029453,-2.2596988127,0.1303572841
 N, -0.9720522758,-2.4757321803,-1.1082314242
 C, 2.6810220589,-2.0001302194,-0.3225862007
 H, 3.2443579206,-2.7329303033,-0.9118089859
 C, -2.1133408278,-2.0705398383,-0.671246347
 H, -2.6088637109,-2.5656825794,0.168039947
 C, 3.3184776357,-0.710332713,-0.0845358002
 C, 4.5806081763,-0.4428493099,-0.6379129746
 C, 2.7069924424,0.2764354785,0.7155216813
 C, 5.2488062893,0.7639242601,-0.4405690922
 H, 5.0298023587,-1.221899588,-1.2412811513
 C, 3.3649304278,1.4831350573,0.9433243409
 C, 4.6069055302,1.7171579855,0.3679828436
 H, 2.9029205925,2.2256108179,1.583039662
 H, 5.0880688337,2.6677667366,0.5646478857
 C, -2.7739982677,-0.9016874492,-1.2237453692
 C, -3.9955339512,-0.4773265202,-0.6671564869
 C, -2.1910069867,-0.152085844,-2.2733802377
 C, -4.6608844958,0.6596513548,-1.105571575

H, -4.3787414666,-1.0509236861,0.1653555162
 C, -2.8630268247,0.9826524335,-2.7401389106
 C, -4.0645471897,1.3703918476,-2.1660283535
 H, -2.4189926308,1.5477092848,-3.5512683174
 H, -4.5458372349,2.2627261287,-2.5514722766
 O, 1.4875990652,0.0779486195,1.2984298956
 H, 1.1394185725,-0.8390069109,1.0623758054
 O, -1.0004785027,-0.4753890882,-2.8108117899
 H, -0.6901102524,-1.2972381404,-2.3469865563
 C, -5.9502203073,1.1752399992,-0.4450922938
 C, -7.0598140051,1.3450150804,-1.5062768973
 H, -7.977202384,1.7166118348,-1.0395851086
 H, -6.7764296652,2.0549536939,-2.28756864
 H, -7.2876185605,0.3904546478,-1.9886702846
 C, -6.4602283291,0.2150207415,0.645797696
 H, -7.3738708373,0.6190656297,1.09073663
 H, -6.7015185013,-0.7696182263,0.234674823
 H, -5.7278887671,0.0832614371,1.445923043
 C, -5.6556781688,2.5407085437,0.2203596529
 H, -4.8746877306,2.4322428985,0.9774429004
 H, -5.3237701909,3.2831559817,-0.5108084789
 H, -6.5548178301,2.9309250745,0.7076526397
 C, 6.6257312164,1.0729490447,-1.0523038257
 C, 7.6451104575,1.3283038564,0.0821966423
 H, 7.7453995268,0.448649548,0.7236736247
 H, 8.6289519988,1.557073135,-0.3377955584
 H, 7.3496009631,2.1702229983,0.7126388108
 C, 7.1496824776,-0.0852508104,-1.9203347744
 H, 7.2805213616,-1.0031903611,-1.3405913654
 H, 6.4833425321,-0.2992536923,-2.7605927231
 H, 8.1250740702,0.1808215683,-2.3351302019
 C, 6.5197486745,2.3335200105,-1.9419452765
 H, 6.1956644814,3.2081398962,-1.3732486175
 H, 7.492793,2.5672760293,-2.3835773115
 H, 5.8055682072,2.1793830314,-2.7552003248
 C, -2.0259385004,-0.2389226393,2.1059542771
 O, -0.8760258007,-0.6301813163,1.7607686346
 O, -3.035034657,-0.842609263,2.396822707

Zero-point correction=	0.628389 (Hartree/Particle)
Thermal correction to Energy=	0.667644
Thermal correction to Enthalpy=	0.668589
Thermal correction to Gibbs Free Energy=	0.553847
Sum of electronic and zero-point Energies=	-2187.290597
Sum of electronic and thermal Energies=	-2187.251342

Sum of electronic and thermal Enthalpies= -2187.250397

Sum of electronic and thermal Free Energies= -2187.365139

TSJ'-K'

C, -0.6681168856,1.4588390027,0.7827845776
C, 0.1835610641,1.6841628898,-0.4583262604
H, -0.6227965511,0.4056226289,1.0633802088
H, 0.9490022575,2.4386041165,-0.4439960296
H, -0.2157562688,1.3848129216,-1.4115799036
O, -2.0266560793,1.7398472305,0.5163816162
C, -0.2407990181,2.317949016,1.9752978758
H, -0.9316441751,2.1642107167,2.7995038591
H, -0.2052965919,3.3678817308,1.6973854531
Cl, 1.4182789644,1.8840611137,2.6081152405
C, -0.6662443036,-5.6636889766,1.7945852207
C, 0.69413337,-5.527434939,2.0681564252
C, 1.3850528174,-4.415624094,1.6010064633
C, 0.7221727917,-3.4439157921,0.8509635448
C, -0.6633560332,-3.5532843811,0.5885396278
C, -1.3352443544,-4.6882831408,1.065002125
H, -1.2065811208,-6.5343157389,2.1470837369
H, 1.2144924299,-6.2777982168,2.6504265962
H, 2.4318149324,-4.2901185846,1.8500737121
H, -2.3835003891,-4.8157318331,0.8235227196
N, 1.3799593156,-2.2959731163,0.3569436836
N, -1.26495016,-2.5626667657,-0.1912146321
C, 2.6650197172,-2.1550358937,0.0998035869
H, 3.2912634233,-3.026952945,0.2610011874
C, -2.486178029,-2.1802257404,0.0400910695
H, -3.0287738723,-2.562235023,0.9121522813
C, 3.2716012118,-0.9815568112,-0.3903328811
C, 4.6671086679,-1.0248921077,-0.6750696348
C, 2.519889221,0.2275767155,-0.6241515206
C, 5.351315551,0.0516131256,-1.187095485
H, 5.1817097407,-1.9568468915,-0.473600584
C, 3.2367099614,1.3218233771,-1.1691328626
C, 4.5841564,1.2234705683,-1.4306649485
H, 2.7186638369,2.2428126605,-1.3938982844
H, 5.0764007364,2.0944600659,-1.8487778191
C, -3.1869529204,-1.238021459,-0.7815447466
C, -4.4731138736,-0.801472537,-0.3851922847
C, -2.6105696857,-0.7020144311,-1.960631493
C, -5.1934701645,0.136445673,-1.1003162547
H, -4.872544959,-1.2139448067,0.5328219259
C, -3.3420743854,0.2218487098,-2.7081520955

C, -4.5904391525,0.631014079,-2.2778151624
 H, -2.8954725134,0.6329159982,-3.6050481853
 H, -5.1085918075,1.379499231,-2.8643253207
 O, 1.2524376836,0.2383891856,-0.3328440406
 O, -1.3759798343,-1.0391048692,-2.377082699
 H, -1.0112421913,-1.682893307,-1.727430923
 C, -6.5688884017,0.6646311901,-0.6635186726
 C, -6.9862431343,0.1128228444,0.7114508478
 H, -7.9621593828,0.5204840488,0.9874064436
 H, -7.0772223155,-0.9778485394,0.7082241838
 H, -6.2756823108,0.4005648237,1.4910762699
 C, -6.5191480342,2.2078959654,-0.5701019304
 H, -7.4635375919,2.5866505968,-0.1663102817
 H, -5.6927979402,2.5418300763,0.0594255954
 H, -6.3719148158,2.6682161311,-1.5496683572
 C, -7.6327463545,0.2404695315,-1.7022257962
 H, -7.3967649435,0.624208605,-2.6980542868
 H, -7.705275785,-0.849115449,-1.7711795961
 H, -8.6158174441,0.6305953054,-1.4205333242
 C, 6.8538555388,0.0401766133,-1.5056802709
 C, 7.562387399,1.1413918355,-0.6829890888
 H, 7.4369551625,0.9705773448,0.3894898991
 H, 8.6337299261,1.1486086954,-0.9039544032
 H, 7.172319737,2.1363595257,-0.9102688585
 C, 7.5049281678,-1.311707574,-1.1633260133
 H, 7.4123269011,-1.5500394264,-0.0999043723
 H, 7.0691989115,-2.1315504137,-1.7414896368
 H, 8.5714024619,-1.276263655,-1.3991799334
 C, 7.0623249699,0.3106073965,-3.0140071888
 H, 6.654826081,1.27846913,-3.3158689079
 H, 8.1295476827,0.3123051717,-3.2540013912
 H, 6.5783615191,-0.4599124439,-3.6200945426
 C, -2.1919527588,2.9268098958,-0.3043579845
 O, -3.3321318714,3.3100238088,-0.4446366561
 O, -1.0835261129,3.3506059357,-0.7444699403
 H, 0.8058478248,-1.4768513557,0.1272731576

Zero-point correction=	0.631681 (Hartree/Particle)
Thermal correction to Energy=	0.670665
Thermal correction to Enthalpy=	0.671609
Thermal correction to Gibbs Free Energy=	0.557560
Sum of electronic and zero-point Energies=	-2187.326358
Sum of electronic and thermal Energies=	-2187.287374
Sum of electronic and thermal Enthalpies=	-2187.286430
Sum of electronic and thermal Free Energies=	-2187.400478

TSI-L

C, 1.8466209258,2.8041421349,-1.03281731
C, 2.989291721,1.8804682835,-1.4520176403
H, 2.1972059426,3.4298043951,-0.2008678812
H, 3.8827430617,2.435613774,-1.7494057602
H, 2.6587924189,1.2349989577,-2.2716316192
O, 0.726217706,2.03083824,-0.6576381066
C, 1.3487419189,3.7042791534,-2.1569630461
H, 0.5148788233,4.3025595424,-1.8009673742
H, 1.0409163539,3.1210053246,-3.0231587972
Cl, 2.6231329082,4.8710504339,-2.7256309411
C, -0.8140029197,1.3849114277,5.1577217202
C, 0.5514734982,1.1344933423,5.2494062861
C, 1.2688443788,0.7927435142,4.106612927
C, 0.6433089205,0.7044268986,2.8566351973
C, -0.7426121665,0.9706555946,2.7621324187
C, -1.4522507528,1.2980672361,3.9235171432
H, -1.3816472627,1.6618854502,6.0385629667
H, 1.0627038997,1.2182583823,6.2013984703
H, 2.3385317446,0.6275762715,4.1644421247
H, -2.5094827007,1.5211636726,3.8377310016
N, 1.3679155967,0.3842760292,1.6923897595
N, -1.3788820916,0.9380116358,1.5095369891
C, 2.1552360613,-0.6263644528,1.7195234888
H, 2.1620260713,-1.2829396823,2.5997069699
C, -2.3769741452,0.1574790611,1.3437856222
H, -2.6711814727,-0.5392849916,2.1413611394
C, 3.0446047609,-1.0681939071,0.6409479982
C, 3.4294506649,-2.4204003253,0.6382147996
C, 3.5251985614,-0.228442737,-0.3837566279
C, 4.209658073,-2.9864214227,-0.3677574549
H, 3.0692992451,-3.0362399872,1.4532985881
C, 4.3055471568,-0.7755905834,-1.4038155664
C, 4.6273494873,-2.1268746995,-1.3953992583
H, 4.6838792025,-0.1357362952,-2.1916880616
H, 5.2395526365,-2.5088907108,-2.2043340139
C, -3.2115737785,0.0803127501,0.1449209625
C, -4.1556496982,-0.9562536872,0.0885025819
C, -3.1486659892,0.9876065015,-0.9380816921
C, -5.0392362096,-1.1375172261,-0.9774012918
H, -4.1848952249,-1.6414324679,0.9296544767
C, -4.0282226661,0.8269120911,-2.0059900073
C, -4.9534371856,-0.2118948221,-2.0246011782
H, -3.9712438581,1.5332673076,-2.8252374755

H, -5.6119988123,-0.2910341539,-2.879549934
 O, 3.2648205355,1.0943762833,-0.2839638492
 H, 0.964246903,1.4763088876,0.11584674
 O, -2.2795960908,2.0253739783,-0.9778096525
 H, -1.4190348527,2.5378532873,-0.1434693479
 C, -6.0429179506,-2.3040772381,-0.9642707555
 C, -6.9676951793,-2.1779797331,0.2684092464
 H, -7.6834372292,-3.0053616981,0.2931415007
 H, -6.4035357662,-2.1990122238,1.2038147044
 H, -7.530868701,-1.241390789,0.2387175496
 C, -6.9253884411,-2.3232451857,-2.2257279433
 H, -7.6203661826,-3.1653925663,-2.1738409117
 H, -7.5198916788,-1.4104782268,-2.3198096678
 H, -6.3317766986,-2.4418103129,-3.1363034718
 C, -5.2748264372,-3.6444983984,-0.8936971489
 H, -4.6124124811,-3.7605432986,-1.755743516
 H, -4.6631651462,-3.7149695684,0.0088518798
 H, -5.9758883364,-4.4848226722,-0.8869921583
 C, 4.618382895,-4.4696609621,-0.3845459149
 C, 6.1606806512,-4.5778760835,-0.3605134888
 H, 6.5700796905,-4.1139326575,0.5409131107
 H, 6.468857613,-5.6277565176,-0.3729120699
 H, 6.6160218473,-4.0880437225,-1.2243269453
 C, 4.065457355,-5.2397730194,0.8283237626
 H, 4.4360615461,-4.8317736175,1.7728386573
 H, 2.9723211568,-5.2293942744,0.8539530251
 H, 4.3831605236,-6.2842918976,0.7749740222
 C, 4.0769029488,-5.139573402,-1.6687064777
 H, 4.4729174768,-4.668150213,-2.5712456427
 H, 4.3596434835,-6.1963566741,-1.6946404113
 H, 2.9861206111,-5.0780666266,-1.7106767193
 C, -2.6501615063,3.6767050964,-0.4727414922
 O, -3.63906731,4.1903919323,-0.8147798121
 O, -1.5788907246,3.7229918801,0.1512718144

Zero-point correction=	0.625514 (Hartree/Particle)
Thermal correction to Energy=	0.665402
Thermal correction to Enthalpy=	0.666346
Thermal correction to Gibbs Free Energy=	0.548918
Sum of electronic and zero-point Energies=	-2187.308568
Sum of electronic and thermal Energies=	-2187.268680
Sum of electronic and thermal Enthalpies=	-2187.267735
Sum of electronic and thermal Free Energies=	-2187.385163

TSL-M

C, 1.8439509339,3.2267231542,-0.5577575338

C, 2.7713084433,2.2484203756,-1.2776433895
H, 2.3971728151,3.6154974063,0.3057350285
H, 3.6716513308,2.7285637808,-1.6662819619
H, 2.2241805984,1.7255186713,-2.0614984241
O, 0.7420287671,2.5202699747,-0.0248150423
C, 1.4233115928,4.4353678741,-1.3994591368
H, 0.6348315867,4.9767135176,-0.8837654015
H, 1.0983412813,4.1697342539,-2.397483204
Cl, 2.8262029896,5.6020657062,-1.5789749185
C, -0.6612783876,1.954992168,5.4674843576
C, 0.724940735,1.8250563532,5.4776707372
C, 1.3931551231,1.4548058917,4.3119433935
C, 0.6712530876,1.2167596071,3.1466363354
C, -0.7351713257,1.3299522417,3.129997224
C, -1.3889377879,1.7081861579,4.3048393277
H, -1.1831893076,2.2516650702,6.3699841185
H, 1.2881435187,2.0261946816,6.380642468
H, 2.4744932707,1.3794308049,4.2941115758
H, -2.4674952583,1.8108424541,4.2923106119
N, 1.3308456708,0.8437576301,1.928013794
N, -1.3668232613,1.088149443,1.9086532164
C, 2.0228345335,-0.2504009381,1.8435821832
H, 2.0153214035,-0.87921619,2.7329130771
C, -2.0210216359,0.0119226656,1.6817918014
H, -2.2542677939,-0.6832068102,2.502086889
C, 2.7175718921,-0.7840591562,0.699491976
C, 2.9013776792,-2.1841998938,0.6618132712
C, 3.1495091368,0.0012260621,-0.3942726468
C, 3.4013599922,-2.8357443268,-0.4564153512
H, 2.5941753344,-2.7528039536,1.5307654069
C, 3.6407029226,-0.6420936564,-1.532084298
C, 3.7474201602,-2.0242619178,-1.5553776029
H, 3.957778821,-0.0543046999,-2.3841224717
H, 4.1371799582,-2.4861546263,-2.4551796328
C, -2.4236819686,-0.3990680813,0.3415888034
C, -3.5616532923,-1.2122114074,0.1832727001
C, -1.6220705321,-0.0778970556,-0.782505127
C, -3.9904999536,-1.6560535081,-1.0621355194
H, -4.1217953563,-1.4688225083,1.0750528575
C, -2.0446797452,-0.5369282726,-2.037904293
C, -3.2015474518,-1.2868806089,-2.1696159157
H, -1.4405325426,-0.2751306266,-2.8975314839
H, -3.4941520632,-1.6060548904,-3.1640201045
O, 3.1487620434,1.3260681813,-0.2201473016

H, 1.1278884472,1.4805424262,1.0587556615
 O, -0.4529274628,0.5718558275,-0.6437205267
 H, -1.5548753792,2.4092547962,0.3701307362
 C, -5.2539645004,-2.5089284447,-1.2672619319
 C, -5.9720199632,-2.8164997884,0.059373317
 H, -6.8611660664,-3.4222837845,-0.1352516617
 H, -5.3335844542,-3.379693752,0.7460906318
 H, -6.2998544582,-1.9040827236,0.5650632263
 C, -6.2418116235,-1.7505309464,-2.1841229361
 H, -7.1485612966,-2.3430997805,-2.3415399505
 H, -6.5312435267,-0.7954496118,-1.7378231127
 H, -5.8062571063,-1.5409353394,-3.1637150466
 C, -4.8705922472,-3.8530786209,-1.9287371133
 H, -4.3970176679,-3.7059041921,-2.9021785205
 H, -4.172491256,-4.4117020724,-1.2989968677
 H, -5.7612143996,-4.4706240223,-2.0817526828
 C, 3.5752707066,-4.361420775,-0.5411591776
 C, 5.060141433,-4.6960614437,-0.8150337221
 H, 5.700513786,-4.3206024452,-0.0122655558
 H, 5.197639017,-5.7793248481,-0.8810664797
 H, 5.4102146125,-4.2611403671,-1.754108057
 C, 3.156550706,-5.0660975628,0.7614979874
 H, 3.7546724337,-4.7341968083,1.6150042333
 H, 2.1005609971,-4.9013194128,0.9927017618
 H, 3.303819617,-6.1439702959,0.6581026441
 C, 2.7022592662,-4.9123697177,-1.6924717245
 H, 2.9820012485,-4.4827875719,-2.6572806138
 H, 2.8158467958,-5.9978722839,-1.7675119051
 H, 1.6455000239,-4.6905202376,-1.5226328125
 C, -0.4396202347,2.0788275144,-1.114071068
 O, -0.1370719297,2.2493244014,-2.2799107251
 O, -1.5478492762,2.6645551941,-0.569778711

Zero-point correction=	0.630627 (Hartree/Particle)
Thermal correction to Energy=	0.668567
Thermal correction to Enthalpy=	0.669511
Thermal correction to Gibbs Free Energy=	0.560310
Sum of electronic and zero-point Energies=	-2187.298854
Sum of electronic and thermal Energies=	-2187.260914
Sum of electronic and thermal Enthalpies=	-2187.259970
Sum of electronic and thermal Free Energies=	-2187.369171

TSN-K

C, 1.0033242938,4.0052561698,-0.5036608672
 C, 1.3362069328,2.6134149331,-0.8621613646
 H, 1.9024478054,4.6254481844,-0.6244837349

H, 1.7056821711,2.4417464749,-1.8641776316
H, 0.8826834661,1.7764834848,-0.3453869602
O, 0.443392659,4.1288742809,0.7717369272
C, -1.0645785176,-0.4290761188,4.4912930115
C, 0.3197718136,-0.4650495544,4.6307959444
C, 1.1339371339,-0.3322126508,3.5110875904
C, 0.5821971182,-0.1557410093,2.2372805822
C, -0.8230412047,-0.1022128117,2.0990864371
C, -1.6292187526,-0.2488692737,3.2327586139
H, -1.705034867,-0.5114518871,5.3615102625
H, 0.7682119944,-0.5710169404,5.6114866486
H, 2.2115593014,-0.3095557784,3.6191080793
H, -2.7047070395,-0.1708968775,3.123331559
N, 1.389017311,0.0007023179,1.0959760467
N, -1.3742655003,0.1331538198,0.827091283
C, 2.3434127755,-0.8237735463,0.8947139713
H, 2.4707141607,-1.7035022246,1.5395778403
C, -2.3509394952,-0.574760395,0.3786772099
H, -2.7295683736,-1.4341767836,0.9439871685
C, 3.2904131437,-0.7386929385,-0.2243220338
C, 3.8346451824,-1.9508549115,-0.6868639117
C, 3.6767080945,0.4521961441,-0.8700260792
C, 4.6726773041,-2.0414936989,-1.7951483251
H, 3.5521956257,-2.8481100033,-0.1505885311
C, 4.5116683811,0.3810424342,-1.9882684325
C, 4.9879967954,-0.8363881805,-2.4454779164
H, 4.7999923478,1.3092049039,-2.4671126235
H, 5.6371335513,-0.8411059302,-3.3131955417
C, -2.9901293385,-0.2914089761,-0.8933103585
C, -4.0193803413,-1.1296963588,-1.3631190879
C, -2.5880393082,0.8139489172,-1.6785498983
C, -4.664093424,-0.9153528713,-2.5746499929
H, -4.3010665575,-1.965598316,-0.7341438747
C, -3.2251090973,1.0415640872,-2.9006663068
C, -4.232643697,0.1933454553,-3.3302899729
H, -2.9141497256,1.8890019351,-3.499794294
H, -4.7019879567,0.4051262186,-4.2842140074
O, 3.328504354,1.7079913074,-0.4748893108
H, 3.0111011391,1.8364071141,0.4593182981
O, -1.62152286,1.6573152748,-1.2661367313
H, -1.3211927738,1.3268675018,-0.3718457278
C, -5.7967988819,-1.813115622,-3.1009195995
C, -7.0796749909,-0.9689651102,-3.2840374631
H, -7.8951144193,-1.5925061166,-3.6632080083

H, -7.3988457894,-0.5324160876,-2.3337875213
 H, -6.9303529553,-0.1512761228,-3.9931508604
 C, -5.3859286078,-2.4211115474,-4.4619921893
 H, -6.1845282819,-3.0608461134,-4.849829467
 H, -5.1877290784,-1.6490613398,-5.2091746045
 H, -4.4821830775,-3.0280971728,-4.36087416
 C, -6.1171490324,-2.9691156781,-2.1362043509
 H, -5.2562695982,-3.6275623158,-1.9899021182
 H, -6.4419236708,-2.6042907953,-1.1578235185
 H, -6.9287393519,-3.5757635932,-2.5461567056
 C, 5.2470874541,-3.3720995274,-2.3089677577
 C, 6.7918684994,-3.3170032533,-2.2557528153
 H, 7.1420439666,-3.1575287432,-1.2324402346
 H, 7.2166377653,-4.2576944407,-2.6185573001
 H, 7.191372348,-2.5107670372,-2.8751722405
 C, 4.7789901328,-4.573270288,-1.4677987439
 H, 5.0979109717,-4.4900397252,-0.4251361111
 H, 3.6914662908,-4.6854350424,-1.4878699097
 H, 5.2114208296,-5.4929056515,-1.8702469076
 C, 4.7919937234,-3.5981832614,-3.7695336388
 H, 5.1316432421,-2.7971725726,-4.4302170267
 H, 5.1994275864,-4.5390225804,-4.1514352615
 H, 3.7018584082,-3.6477049518,-3.8362420363
 C, 1.2419607762,3.538040164,1.8206860206
 O, 0.8600110985,3.7220511197,2.9456792919
 O, 2.2449248809,2.9136974681,1.3517538029
 C, -0.0777364431,4.5521618736,-1.4754461192
 H, -0.9263218935,3.8784544898,-1.5448792066
 H, -0.3820418963,5.5256470399,-1.1023185479
 Cl, 0.5721567891,4.7951591723,-3.1505912485

Zero-point correction=	0.627386 (Hartree/Particle)
Thermal correction to Energy=	0.666760
Thermal correction to Enthalpy=	0.667704
Thermal correction to Gibbs Free Energy=	0.551336
Sum of electronic and zero-point Energies=	-2187.282127
Sum of electronic and thermal Energies=	-2187.242753
Sum of electronic and thermal Enthalpies=	-2187.241809
Sum of electronic and thermal Free Energies=	-2187.358177

TSG⁻H⁺

C, 0.2016867243,-2.1561485708,0.5436384492
 C, -0.9610294919,-2.1597979926,-0.3285624066
 H, 0.3696405922,-1.2256318819,1.0878114368
 H, -1.2040425302,-1.2312594498,-0.8116225596
 H, -1.2993783342,-3.0967399933,-0.7368144088

O, 0.8358569107,-2.2699233397,-0.7070385921
C, 0.5302654425,-3.3851903203,1.3697813345
H, 1.612844798,-3.4769271319,1.4432186774
H, 0.1131731826,-4.2873823244,0.9272482386
Cl, -0.0869881262,-3.3187349742,3.0911231528
C, 0.4920338449,4.1215929573,2.063130099
C, -0.8208401714,3.8844245913,2.4554467533
C, -1.4879124503,2.761058069,1.9770002138
C, -0.8770588574,1.8394121169,1.106739617
C, 0.4873554657,2.0494492065,0.7569034539
C, 1.1268182943,3.2102435811,1.2237433578
H, 1.0203902877,5.007783048,2.3987044318
H, -1.3306444625,4.5711626595,3.1234714425
H, -2.5022545313,2.5564093886,2.2993803794
H, 2.132920184,3.4179697943,0.8780992215
N, -1.5724667369,0.7122120476,0.6705114081
N, 1.1403304929,1.1765556358,-0.1330702876
C, -2.7716878939,0.8828684031,0.2296686882
H, -3.1282899838,1.9141553973,0.0701154809
C, 2.3892501842,0.958514348,0.0486311527
H, 2.8844744959,1.3327816343,0.958704724
C, -3.7760869629,-0.1107197548,-0.0936039894
C, -4.9631457539,0.4005510953,-0.6742563652
C, -3.6931478264,-1.517083858,0.2361585403
C, -6.0829265245,-0.3613592976,-0.9606921759
H, -4.9690016768,1.4633434579,-0.8928798156
C, -4.8797773736,-2.2768718777,-0.0402031438
C, -6.0053851857,-1.7319655011,-0.6096843343
H, -4.8409408088,-3.3287674246,0.2234557213
H, -6.8562888917,-2.3826590999,-0.7950298748
C, 3.3285978688,0.3439477638,-0.8937713226
C, 4.6905882285,0.5681171771,-0.6267285745
C, 2.9741266824,-0.3156676705,-2.1034646218
C, 5.7206726013,0.2429469277,-1.509351163
H, 4.9298772982,1.0554983803,0.3142134079
C, 4.003146523,-0.6081697333,-3.0101729462
C, 5.3344447953,-0.3342587973,-2.7274588361
H, 3.7193718912,-1.0913646081,-3.9381405171
H, 6.0788392512,-0.6011002624,-3.4677611515
O, -2.6784986848,-2.0999858342,0.7532644428
O, 1.7314022402,-0.65971865,-2.4263700318
H, 1.2737276212,-1.1297916319,-1.6425818949
C, 7.186009393,0.5339535113,-1.1373194792
C, 7.5565704688,-0.2264784497,0.1570055191

H, 8.5952984176,-0.0233671157,0.440800395
 H, 6.9172369464,0.0667261588,0.9926752153
 H, 7.4438670684,-1.3050475405,0.0172243146
 C, 8.1648905831,0.0946506795,-2.2422112766
 H, 9.1919522236,0.3118799258,-1.9332372935
 H, 8.0966923603,-0.9788049769,-2.4390770571
 H, 7.9812799757,0.6254186397,-3.1805181489
 C, 7.3778298527,2.0510588272,-0.9074065395
 H, 7.1320736243,2.6132849173,-1.8125971611
 H, 6.73637986,2.4197704594,-0.10378391
 H, 8.4162893326,2.272907287,-0.6366472962
 C, -7.3582264439,0.1988988359,-1.6102836288
 C, -8.5700224364,-0.0231482377,-0.6745321056
 H, -8.4193823333,0.4916649971,0.2784055646
 H, -9.4899949252,0.3602655381,-1.1315287062
 H, -8.7208920561,-1.0833461739,-0.4576159125
 C, -7.2547043559,1.7074851132,-1.8989873971
 H, -7.1004271671,2.2837246678,-0.9825645414
 H, -6.4315177287,1.9317736998,-2.582635564
 H, -8.1808282305,2.0609884444,-2.3636788887
 C, -7.6212208564,-0.5246306206,-2.9525151676
 H, -7.7331637026,-1.60226674,-2.8104294436
 H, -8.5372535548,-0.149804255,-3.4242078621
 H, -6.7890306878,-0.3664825127,-3.6439552712

Zero-point correction=	0.598678 (Hartree/Particle)
Thermal correction to Energy=	0.635468
Thermal correction to Enthalpy=	0.636413
Thermal correction to Gibbs Free Energy=	0.526783
Sum of electronic and zero-point Energies=	-1998.164461
Sum of electronic and thermal Energies=	-1998.127671
Sum of electronic and thermal Enthalpies=	-1998.126726
Sum of electronic and thermal Free Energies=	-1998.236356

TSI-J

C, -0.5580314161,-2.6196743799,-1.1659482726
 C, -1.2328201594,-1.2382533069,-1.1946382636
 H, -1.1180150984,-3.2505271619,-0.467139089
 H, -1.2889077177,-0.8268507818,-2.2089835139
 H, -0.6692122745,-0.5720813332,-0.5479732634
 O, 0.7758345852,-2.518678258,-0.7522425459
 C, -0.4972902814,-3.3160580406,-2.5287431199
 H, -0.0721281471,-4.3088273018,-2.4135162698
 H, 0.0865994727,-2.7270878151,-3.2336223685
 Cl, -2.1413433202,-3.5782791327,-3.3398095398
 C, 1.1214354109,-1.353637698,4.9216656424

C, -0.2528213759,-1.226194989,5.1107773102
C, -1.062486712,-0.846901385,4.043610051
C, -0.5149943228,-0.5819368805,2.7813045211
C, 0.8915754466,-0.6606538976,2.5969756617
C, 1.6830557293,-1.0769317315,3.6785651289
H, 1.7550618284,-1.6957986512,5.733141052
H, -0.6991073701,-1.4582263522,6.0719367523
H, -2.1403322303,-0.8143040104,4.1586258872
H, 2.7421923625,-1.233528087,3.5156204732
N, -1.3138076895,-0.347626927,1.6659045012
N, 1.4054519994,-0.3567992109,1.3377716716
C, -2.287214623,0.4697395104,1.6685744235
H, -2.4832374804,1.1254550684,2.5326810487
C, 2.5443153766,0.2171635279,1.2437849092
H, 3.0683912701,0.5540164208,2.1528411823
C, -3.220815467,0.6394929269,0.5473438644
C, -4.112984768,1.7254188364,0.6220987534
C, -3.3229220697,-0.2443504247,-0.5536780664
C, -5.0842973808,1.9894931759,-0.3403750009
H, -4.0181211918,2.3734784554,1.4855127997
C, -4.3038214332,0.0068808159,-1.5183422046
C, -5.1603847126,1.0937735841,-1.418410989
H, -4.3774377529,-0.6900114868,-2.3450618094
H, -5.9010225392,1.2402722561,-2.1975995622
C, 3.2544789506,0.5548827814,0.0175318312
C, 4.4166761861,1.3333973181,0.1850531449
C, 2.8400997065,0.2159196019,-1.3083271574
C, 5.1879755037,1.8318634239,-0.8597809269
H, 4.7030984577,1.5562623288,1.2092076368
C, 3.612407944,0.7474597513,-2.365019641
C, 4.7389651907,1.5225144782,-2.1549636277
H, 3.2873025993,0.503792919,-3.3701358527
H, 5.2802517899,1.8800580256,-3.0229166199
O, -2.5882442739,-1.3764333158,-0.6831508327
O, 1.7975486706,-0.507253782,-1.6470634603
H, 1.4243007678,-1.3469356822,-1.0711121852
C, 6.4451388274,2.6732452436,-0.5751312253
C, 6.0606221596,3.9420446432,0.2213487986
H, 6.9480905777,4.547891841,0.4374508601
H, 5.3561866668,4.5561290754,-0.3466120607
H, 5.5872027686,3.6897943877,1.1730746388
C, 7.4549840469,1.8438345613,0.2519339259
H, 8.3556843113,2.4305885029,0.4664990199
H, 7.0269427756,1.5253154634,1.2052028701

H, 7.7532796272,0.9441368267,-0.2930840367
 C, 7.147891178,3.1217234088,-1.8697726511
 H, 7.4751146063,2.2670510058,-2.4682680813
 H, 6.4943694121,3.741036806,-2.4905495026
 H, 8.0341016636,3.7151598669,-1.6241254001
 C, -6.0519493784,3.1829427566,-0.2550027938
 C, -5.8110003528,4.0440565075,0.998391583
 H, -4.801472181,4.4634298715,1.0137258161
 H, -6.5176293661,4.8792602167,1.0137016242
 H, -5.9559454935,3.4709850714,1.9182859528
 C, -5.8719494207,4.0852985405,-1.4979084099
 H, -4.8518486488,4.4752432289,-1.5494993053
 H, -6.0655347791,3.5393302497,-2.42411009
 H, -6.5621076295,4.9349638919,-1.4583376153
 C, -7.5084911115,2.6654813221,-0.2082773897
 H, -7.6645523752,2.026288373,0.6650430628
 H, -8.2118876961,3.5031527133,-0.1502864285
 H, -7.7571591938,2.080358649,-1.0966251282
 C, 1.4455877125,-3.8379809127,0.351722017
 O, 0.5951968986,-4.6712359871,0.4362972921
 O, 2.5373635038,-3.4570081877,0.631205953

Zero-point correction=	0.612806 (Hartree/Particle)
Thermal correction to Energy=	0.652385
Thermal correction to Enthalpy=	0.653329
Thermal correction to Gibbs Free Energy=	0.536817
Sum of electronic and zero-point Energies=	-2186.840740
Sum of electronic and thermal Energies=	-2186.801162
Sum of electronic and thermal Enthalpies=	-2186.800218
Sum of electronic and thermal Free Energies=	-2186.916730

TS2J--2K

C, 0.0121408026,2.9748292486,1.3313355616
 C, 1.1083550147,3.0967102289,0.2997740919
 H, -0.224660577,1.9275243511,1.4903224892
 H, 2.0568553801,3.5331431002,0.5531082964
 H, 0.8996052173,2.8381835637,-0.7216025131
 O, -1.1664365452,3.600729605,0.8245417116
 C, 0.3273994434,3.6803421517,2.6524683398
 H, -0.5433386803,3.6315192445,3.301143061
 H, 0.6090433522,4.715105853,2.4727696968
 Cl, 1.70318097,2.9268623392,3.5857865828
 C, -0.444357746,-4.9414265743,2.8552432547
 C, 0.9310382343,-4.7256954141,2.9429090355
 C, 1.504541176,-3.6159567448,2.3326563601
 C, 0.7273035084,-2.6939201946,1.60767674

C, -0.6762204889,-2.9203822365,1.5219901518
C, -1.2366455715,-4.0380619616,2.1552202574
H, -0.9003577719,-5.7903874095,3.3529149809
H, 1.5546756713,-5.4099266209,3.5090379175
H, 2.5650261812,-3.422249886,2.4443330207
H, -2.3115344052,-4.1792113097,2.126974851
N, 1.2542373457,-1.5460079216,1.0332669084
N, -1.4197620475,-1.9528227341,0.847879167
C, 2.3678891131,-1.6157563647,0.3927486876
H, 2.8211918537,-2.6074154372,0.2251097948
C, -2.5915260664,-2.1315805257,0.3496332325
H, -3.0848477869,-3.1133780514,0.3443726246
C, 3.1329178539,-0.5435811521,-0.2054502632
C, 4.2812814809,-0.9503703906,-0.9226378418
C, 2.7939621112,0.8594130807,-0.1304990422
C, 5.1244227734,-0.0847087389,-1.5994889483
H, 4.486808277,-2.0155818917,-0.9315782104
C, 3.6669152132,1.734899005,-0.8541193294
C, 4.7687512092,1.2808464783,-1.544954069
H, 3.4546556806,2.7954771547,-0.8530432605
H, 5.3802115752,2.0159723885,-2.0609901008
C, -3.3314066361,-1.0267062595,-0.2276310827
C, -4.6509320547,-1.2220101753,-0.6838908105
C, -2.7545331432,0.2684207894,-0.3101438966
C, -5.4268666744,-0.1909615121,-1.1938226617
H, -5.0516619396,-2.2269397483,-0.6110737125
C, -3.5378782566,1.3236427258,-0.8045240577
C, -4.8315113044,1.0898411412,-1.2310791333
H, -3.1047124869,2.3172231188,-0.817765041
H, -5.400326337,1.9353626194,-1.6026688928
O, 1.7800125019,1.2767667751,0.5408482138
O, -1.5007195968,0.5252412325,0.0561251189
H, -1.0916642235,-0.3085972956,0.4164575444
C, -6.8692939275,-0.3824899616,-1.6920516428
C, -7.3377490072,-1.8445150894,-1.575997272
H, -8.3643778526,-1.9341975189,-1.9434612721
H, -6.7128341134,-2.5178038254,-2.1693941875
H, -7.3260864363,-2.1925129293,-0.5392835746
C, -7.8299493132,0.4952391411,-0.8561493161
H, -8.8615908015,0.3776796852,-1.2057327769
H, -7.7918807237,0.2130514269,0.1996155383
H, -7.5720774662,1.5543408206,-0.9254213344
C, -6.9654244126,0.0329729299,-3.1786694413
H, -6.6783832632,1.0766757863,-3.3254275964

H, -6.3051819279,-0.5824099603,-3.7960308963	
H, -7.9901615283,-0.0876476629,-3.5466980623	
C, 6.3717615067,-0.534293633,-2.3764535689	
C, 7.6299888125,0.1461716635,-1.7872893036	
H, 7.7619488163,-0.1306283691,-0.7376766116	
H, 8.5286623758,-0.1546289838,-2.3382763829	
H, 7.5568224503,1.2352480397,-1.835769485	
C, 6.582651858,-2.0579010993,-2.3104294022	
H, 6.7159637226,-2.4023436307,-1.2811057888	
H, 5.7386252518,-2.6013714529,-2.7439078556	
H, 7.4804128473,-2.3333126869,-2.8728358686	
C, 6.2353258823,-0.1369911576,-3.8652752525	
H, 6.1145126383,0.9424834028,-3.9837912497	
H, 7.1241316536,-0.4391486635,-4.4312138844	
H, 5.3623663189,-0.618670512,-4.3143457015	
C, -0.8564499052,4.748649892,0.0466859388	
O, -1.7887622566,5.4090879396,-0.358698473	
O, 0.4054581405,4.8932422941,-0.1130966714	
Zero-point correction=	0.616295 (Hartree/Particle)
Thermal correction to Energy=	0.655326
Thermal correction to Enthalpy=	0.656270
Thermal correction to Gibbs Free Energy=	0.541260
Sum of electronic and zero-point Energies=	-2186.817234
Sum of electronic and thermal Energies=	-2186.778204
Sum of electronic and thermal Enthalpies=	-2186.777260
Sum of electronic and thermal Free Energies=	-2186.892270

cis-G'

C, -0.044361862,-3.3518248763,2.7502690869
 C, -0.1725191847,-3.4029823192,1.2928784191
 H, -0.3452593861,-2.4389066983,3.257092328
 H, -0.5566473547,-2.5289239595,0.7712745459
 H, -0.2847666985,-4.3698430718,0.8103194997
 O, 1.128864285,-3.2146000494,1.9202063079
 C, -0.0348634619,-4.5993076923,3.5879210344
 H, 0.5783268917,-4.4779845431,4.4792277354
 H, 0.3158481878,-5.452719327,3.0113805531
 Cl, -1.7118967754,-4.9889952457,4.1691311212
 C, 0.7387426765,5.5692243667,1.2677500431
 C, -0.6417151951,5.6066329069,1.0858678605
 C, -1.3300887339,4.4472897922,0.7428925662
 C, -0.6463916621,3.2438769013,0.5534829923
 C, 0.7591142954,3.1971918441,0.7253530568
 C, 1.4265667907,4.3730685218,1.0971086375

H, 1.2754911246,6.4632564245,1.5632274049
H, -1.1903222007,6.5282411943,1.2398427964
H, -2.4090446419,4.4776889923,0.6559376307
H, 2.4928672925,4.3273703226,1.2845965114
N, -1.3046905293,2.0519946336,0.1947895237
N, 1.385323299,1.9602650751,0.5931165017
C, -2.5040367397,1.971085546,-0.3768709253
H, -2.9690571605,2.9145770204,-0.6458681274
C, 2.5419714246,1.8731056509,0.0505096795
H, 3.011676414,2.7613574225,-0.398311617
C, -3.1906467608,0.7936677312,-0.6658046109
C, -4.4723764803,0.8854375936,-1.2982747905
C, -2.6183950658,-0.5094125334,-0.3278377465
C, -5.2242010555,-0.2147691115,-1.608350956
H, -4.8369227123,1.881316596,-1.5249415681
C, -3.4474322074,-1.6434091438,-0.6669660644
C, -4.6627989148,-1.4927769093,-1.2669227575
H, -3.0638839553,-2.628605277,-0.4274042806
H, -5.2323547199,-2.3877013887,-1.4962605347
C, 3.3380819549,0.6597446489,-0.0777347842
C, 4.506400665,0.7382414295,-0.8539666359
C, 3.0043254826,-0.5829237603,0.5178271576
C, 5.3512996688,-0.3443782425,-1.0930284577
H, 4.7411321544,1.7046224669,-1.2890094817
C, 3.8385355837,-1.6802339981,0.2796350661
C, 4.9785639469,-1.5615639279,-0.506583301
H, 3.5819052857,-2.6352915575,0.7256576378
H, 5.5854955284,-2.4457539483,-0.6528505185
O, -1.4901069931,-0.6260484149,0.2118334683
O, 1.9206135899,-0.6670740661,1.2999145404
H, 1.7589717754,-1.5939005595,1.5709757767
C, 6.6151208045,-0.1717226901,-1.9545431724
C, 7.5478561473,0.8736731616,-1.2999434499
H, 8.4538428276,1.0066333996,-1.8996111003
H, 7.062932561,1.8486986216,-1.2099089691
H, 7.8464947821,0.5559320368,-0.29725473
C, 7.4009829701,-1.4877196451,-2.1010962081
H, 8.2878878934,-1.3188204928,-2.7176931801
H, 7.7394639677,-1.8690851852,-1.1338435235
H, 6.8050513736,-2.2653069547,-2.586825343
C, 6.2204057701,0.3116109738,-3.369095416
H, 5.5634585395,-0.4121738379,-3.8588880131
H, 5.6962597017,1.2697622969,-3.3388394491
H, 7.1115306135,0.4395423358,-3.9917259027

C, -6.6025720666,-0.1514173086,-2.2826995042
 C, -7.6610312262,-0.804482894,-1.3629266709
 H, -7.7227500576,-0.277487976,-0.4069554788
 H, -8.6482733993,-0.7733934923,-1.8345265844
 H, -7.4284598692,-1.8509751704,-1.151789001
 C, -7.0431004592,1.2957307348,-2.5656635909
 H, -7.1245235226,1.8814233065,-1.645777575
 H, -6.348702234,1.8064125075,-3.2386261208
 H, -8.0259943754,1.2951013023,-3.044551114
 C, -6.5568897262,-0.9117433514,-3.6289328929
 H, -6.2839198722,-1.9612330708,-3.4950885483
 H, -7.5363695925,-0.8832217619,-4.1166804936
 H, -5.8256222893,-0.4606318739,-4.3050722676
 H, -0.8350671269,1.1514125682,0.3733879749

Zero-point correction=	0.615718 (Hartree/Particle)
Thermal correction to Energy=	0.653543
Thermal correction to Enthalpy=	0.654488
Thermal correction to Gibbs Free Energy=	0.539121
Sum of electronic and zero-point Energies=	-1998.732711
Sum of electronic and thermal Energies=	-1998.694886
Sum of electronic and thermal Enthalpies=	-1998.693942
Sum of electronic and thermal Free Energies=	-1998.809309

***cis*-TSG'-H'**

C, 0.0635237989,-2.9594667606,2.8087967176
 C, -0.9896426365,-2.0158568752,3.2098954663
 H, 1.0547066095,-2.6731589589,3.1932264662
 H, -0.7653270151,-1.1171582629,3.7620910432
 H, -2.0140201787,-2.361104359,3.2305568399
 O, -0.1165493545,-2.7266414353,1.4471254278
 C, -0.2008587705,-4.4231846983,3.1312196066
 H, 0.5487938157,-5.0481752795,2.6496505994
 H, -1.1958210285,-4.7208137677,2.8057000386
 Cl, -0.1091087371,-4.7596006395,4.9270724499
 C, 0.7393327772,5.7984774168,1.9377505435
 C, -0.6554861318,5.8106933649,1.9262666388
 C, -1.3601524632,4.6259573078,1.7343223367
 C, -0.6684097045,3.4337600815,1.5270441792
 C, 0.7491495353,3.4083707631,1.5094400082
 C, 1.4338765775,4.6099342912,1.7403670666
 H, 1.2865775359,6.7167897406,2.1173098201
 H, -1.1951688231,6.7340579568,2.0987073325
 H, -2.44272874,4.6256016617,1.784210069
 H, 2.5167144721,4.6018978562,1.7796533115

N, -1.3207796999,2.1939619824,1.3496018166
N, 1.3107626645,2.1556336253,1.3049203048
C, -2.5029817346,1.9991310195,0.7933438435
H, -2.9953768823,2.8862806978,0.4046029348
C, 2.455931688,1.9814960092,0.7527231179
H, 3.0550647047,2.8399812459,0.4125478354
C, -3.1384035456,0.7593141917,0.6134012564
C, -4.3323519258,0.7204864562,-0.1686995496
C, -2.5858364928,-0.4669316841,1.1599528656
C, -4.9690950191,-0.4520348012,-0.4896200563
H, -4.7173036861,1.6693085367,-0.52439817
C, -3.2277076111,-1.6781228317,0.7551349116
C, -4.3576210301,-1.6546362907,-0.0196882182
H, -2.7614127721,-2.6115154723,1.0393175209
H, -4.7985286589,-2.6066610296,-0.2961034057
C, 3.0580966507,0.6880490247,0.4842206376
C, 4.3870682991,0.6680924122,0.022937199
C, 2.3574715146,-0.5464996236,0.6205968708
C, 5.0765454415,-0.5003514515,-0.2870164393
H, 4.8845065201,1.6274930225,-0.0841196698
C, 3.0436173929,-1.7283215645,0.2961933823
C, 4.3615918411,-1.7008610882,-0.1357676732
H, 2.5113869553,-2.6690164267,0.3852248283
H, 4.8358465336,-2.6463375272,-0.3665380387
O, -1.5854304708,-0.4152580898,1.9515909953
O, 1.0964727239,-0.5409429784,1.0170210253
H, 0.6565588332,-1.4657811785,1.0864368722
C, 6.5369332213,-0.4417731825,-0.7711863714
C, 7.4195012358,0.2132333175,0.3165001874
H, 8.4619651801,0.263679651,-0.0140437457
H, 7.0925965764,1.2309658533,0.5432592715
H, 7.383778604,-0.3626090985,1.2452505327
C, 7.1061167501,-1.841427976,-1.0679259959
H, 8.1415852485,-1.7525796987,-1.4077657339
H, 7.1044246125,-2.4778709419,-0.1787878553
H, 6.5432309444,-2.350848994,-1.8548897882
C, 6.6229262979,0.3946521326,-2.0688710304
H, 6.012392003,-0.0500354681,-2.8593944995
H, 6.273627592,1.4184571081,-1.9145644995
H, 7.6571472298,0.4458906751,-2.4241932391
C, -6.2526467451,-0.5289409802,-1.3299369331
C, -7.3641912627,-1.2241693885,-0.5094220114
H, -7.5861179796,-0.6612480737,0.4013013894
H, -8.283835183,-1.2966292951,-1.098123654

H, -7.0796318022,-2.2371101387,-0.2146716663	
C, -6.7603317648,0.8647524364,-1.7403443207	
H, -6.9914262869,1.4850436929,-0.8696977196	
H, -6.0322940199,1.3964850469,-2.3593506097	
H, -7.6778287686,0.7645433573,-2.3260578251	
C, -5.982616187,-1.3421669497,-2.6175538025	
H, -5.6553728608,-2.3607113807,-2.3958916591	
H, -6.8922674501,-1.4111707512,-3.2220122503	
H, -5.2061283365,-0.8667217965,-3.2226997363	
H, -0.7684248814,1.3591820329,1.5871187067	
Zero-point correction=	0.612967 (Hartree/Particle)
Thermal correction to Energy=	0.649819
Thermal correction to Enthalpy=	0.650763
Thermal correction to Gibbs Free Energy=	0.541404
Sum of electronic and zero-point Energies=	-1998.665088
Sum of electronic and thermal Energies=	-1998.628236
Sum of electronic and thermal Enthalpies=	-1998.627292
Sum of electronic and thermal Free Energies=	-1998.736651

cis-H'

C, -0.2434240107,-2.2569200716,2.0291581176
 C, -1.530286459,-1.5332899864,2.4408801671
 H, 0.5910716241,-1.5588112879,2.1528662145
 H, -1.4260717869,-1.0656311853,3.4196577172
 H, -2.3841020612,-2.2148539088,2.4668183102
 O, -0.3257652795,-2.6851678956,0.6922576609
 C, 0.0117623031,-3.507078463,2.8671344034
 H, 0.9416270903,-3.9711734574,2.5508170918
 H, -0.8052158507,-4.2210831867,2.7708855119
 Cl, 0.1829916425,-3.1529693393,4.6501979763
 C, 0.7857997889,5.6404248299,1.4697280991
 C, -0.6122108943,5.6573152435,1.5587932913
 C, -1.3338602981,4.5029341753,1.2842697885
 C, -0.6508477827,3.3506075497,0.9000706209
 C, 0.7675006633,3.3099053093,0.785625337
 C, 1.4692319176,4.4903624938,1.1035154826
 H, 1.3452033648,6.5386669267,1.7068922349
 H, -1.1284769163,6.5567289717,1.8704919178
 H, -2.4111854801,4.4904492256,1.4055663837
 H, 2.5516145452,4.4942777265,1.06585554
 N, -1.2813951565,2.1206662817,0.6220822179
 N, 1.2524529437,2.0906777296,0.3929797224
 C, -2.4921544126,1.9307371881,0.1781890636
 H, -3.0538368275,2.8255385143,-0.0765889482
 C, 2.4447540795,1.8994891269,-0.0918423021

H, 3.1259338053,2.7527744225,-0.2241856753
C, -3.1168107032,0.6660266259,-0.0646002114
C, -4.187660923,0.6457658621,-0.9901054831
C, -2.7056672937,-0.5469760889,0.5523160682
C, -4.8086945735,-0.5256957639,-1.3875920285
H, -4.4919041951,1.5946859158,-1.4136918505
C, -3.3036362407,-1.7390150626,0.1298526922
C, -4.3170163614,-1.716034189,-0.8144855835
H, -2.9302770494,-2.6821260492,0.4978370655
H, -4.7369374685,-2.6674737529,-1.1197580882
C, 2.9659818015,0.6472692156,-0.5187943424
C, 4.3145841312,0.626461915,-0.9629182503
C, 2.1776675351,-0.5792763404,-0.5395514943
C, 4.9659433099,-0.5094946796,-1.3964445271
H, 4.8476020559,1.5738267623,-0.9431217828
C, 2.8876575617,-1.7449398558,-0.9866115408
C, 4.2002766605,-1.7069499705,-1.3881118661
H, 2.3369248358,-2.6796178013,-0.9996013821
H, 4.6569016153,-2.6344023645,-1.7129735795
O, -1.7966330723,-0.4415309994,1.5336711093
O, 0.9536226378,-0.6324382495,-0.2029376902
H, 0.1692489245,-1.986693561,0.1671422724
C, 6.434893757,-0.4521567669,-1.8571557055
C, 7.3284125858,0.0530561069,-0.7006439126
H, 8.3764281267,0.1026266757,-1.015049222
H, 7.0314272255,1.0513046729,-0.3699342269
H, 7.2620379774,-0.6159998983,0.161644012
C, 6.9616862662,-1.8314926489,-2.2962199445
H, 8.004186674,-1.7435045753,-2.6153857745
H, 6.9266979459,-2.5585795761,-1.4801689245
H, 6.3918220835,-2.2347394006,-3.1378932656
C, 6.5684336345,0.5122225578,-3.058844899
H, 5.9560618993,0.1724407916,-3.898630805
H, 6.2454846778,1.5236021381,-2.8002956206
H, 7.6092489162,0.5688647917,-3.3951160642
C, -5.9487968631,-0.5761672526,-2.4176636216
C, -7.189124267,-1.244781743,-1.7813305607
H, -7.5374898577,-0.6773814798,-0.9140480571
H, -8.006594584,-1.2937896541,-2.5065928823
H, -6.9784912697,-2.2647524671,-1.4515232876
C, -6.354225757,0.8273276664,-2.9024453521
H, -6.7096130783,1.4553200056,-2.0803662745
H, -5.5269360719,1.3417790994,-3.3990926396
H, -7.1681782465,0.7432616486,-3.6267407494

C, -5.4923823436,-1.3998416875,-3.6445093423	
H, -5.2272103731,-2.4238904254,-3.3715332742	
H, -6.2950491496,-1.4511615155,-4.3861275599	
H, -4.6189782883,-0.9444701176,-4.1186235623	
H, -0.5987703602,1.338649553,0.6514790648	
Zero-point correction=	0.617664 (Hartree/Particle)
Thermal correction to Energy=	0.654195
Thermal correction to Enthalpy=	0.655139
Thermal correction to Gibbs Free Energy=	0.546796
Sum of electronic and zero-point Energies=	-1998.732815
Sum of electronic and thermal Energies=	-1998.696284
Sum of electronic and thermal Enthalpies=	-1998.695340
Sum of electronic and thermal Free Energies=	-1998.803683

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C, 0.4389597391,2.7070697683,1.3983672909
 C, 1.4114597862,2.6484904345,0.2153227232
 H, 0.3107034661,1.7184528907,1.8392444564
 H, 2.4069472529,2.9548206298,0.5305097022
 H, 1.0467110992,3.3085749945,-0.5737279595
 O, -0.83498949,3.1890236635,0.9198218824
 C, 0.8555549904,3.7088784937,2.4740889833
 H, 0.0808613659,3.7737189974,3.2335029478
 H, 1.0423173113,4.6966301734,2.0548228904
 Cl, 2.3743525554,3.193113435,3.3190466377
 C, 0.1162994307,-3.6688360966,3.8498769154
 C, -1.2725326624,-3.7429329333,3.804632442
 C, -1.9594936671,-3.1905290793,2.7275636901
 C, -1.2792054434,-2.5601449862,1.6791673982
 C, 0.1359018588,-2.5312212834,1.6973465018
 C, 0.8091723418,-3.0691043599,2.8027961221
 H, 0.6605541688,-4.0718062298,4.6962034407
 H, -1.82296556,-4.222210199,4.6060656829
 H, -3.039667112,-3.2648610569,2.6769049397
 H, 1.8876754803,-2.9754626334,2.8545891122
 N, -1.9639905902,-2.0090112579,0.5825017803
 N, 0.8118295591,-1.884881598,0.6472545925
 C, -2.9868595547,-1.2574218271,0.7920994839
 H, -3.2962826675,-0.9976907952,1.8082844443
 C, 1.9046670085,-2.3826813038,0.2169320189
 H, 2.2950119507,-3.3291763617,0.6176250833
 C, -3.7583765918,-0.6737710464,-0.2877589874
 C, -4.8590488925,0.15508529,0.0188613803
 C, -3.4079741503,-0.8897500712,-1.6406906746

C, -5.6262245783,0.7773130021,-0.9598204159
H, -5.0998465517,0.2808272613,1.0685248911
C, -4.1814966341,-0.2739804201,-2.6362825904
C, -5.251556745,0.5329565761,-2.2998972972
H, -3.9063578392,-0.4391634313,-3.6709159286
H, -5.8164815644,0.9910544744,-3.103828182
C, 2.7578150004,-1.7787709282,-0.8130130042
C, 4.0655447644,-2.2822139936,-0.9415797945
C, 2.3677387909,-0.7547578901,-1.6837877294
C, 4.9856177202,-1.7917717816,-1.8657851589
H, 4.3492675037,-3.0841953748,-0.2718912836
C, 3.2545827419,-0.2589596954,-2.629015433
C, 4.5462085569,-0.7620158402,-2.711257075
H, 2.9155363222,0.5146238287,-3.307592444
H, 5.2137724962,-0.3483337189,-3.4576255617
O, -2.3758299262,-1.6529892681,-2.004897827
H, -1.91648643,-1.9512808467,-1.1779142648
O, 1.0508233156,-0.3078138736,-1.7252670673
C, 6.4201377399,-2.3337010667,-1.9908892583
C, 6.7085685601,-3.4614678657,-0.9832954046
H, 7.7368550952,-3.810007634,-1.109102567
H, 6.60123611,-3.1214559162,0.0503937748
H, 6.0498819968,-4.3212879653,-1.1334816865
C, 6.6358380078,-2.8931309773,-3.4163417209
H, 7.6532132991,-3.2819479025,-3.5205415351
H, 5.9371925382,-3.7074376208,-3.6261637601
H, 6.4941049833,-2.1257668683,-4.18089584
C, 7.4246374888,-1.1867659022,-1.7322542532
H, 7.3022731877,-0.3698306372,-2.4473519904
H, 7.2969742373,-0.7741598659,-0.72789629
H, 8.450819801,-1.5556725312,-1.8209089431
C, -6.8373578467,1.6732982073,-0.6472638748
C, -7.0395294403,1.8679669368,0.8663696717
H, -6.1721977411,2.3416295928,1.3354986045
H, -7.9016499736,2.516713283,1.0416508721
H, -7.2317279687,0.9210088303,1.377907888
C, -6.6373845964,3.0674984863,-1.2867870673
H, -5.7431436695,3.5581656856,-0.8926374678
H, -6.5312416613,3.0070881081,-2.372236959
H, -7.4979775781,3.708899056,-1.0735461478
C, -8.1162843172,1.0251064479,-1.2265955427
H, -8.2913074716,0.0423796005,-0.7805112055
H, -8.9890043888,1.6532705193,-1.0223250744
H, -8.0472615154,0.8922361561,-2.3089012446

C, 0.6471447081,0.8026947657,-1.0775133758
O, 1.6302328,1.3277040132,-0.3234655489
O, -0.4548354336,1.2477465504,-1.2106917937
C, -1.880299475,2.3466915245,1.0280810863
O, -1.9140330679,1.3555310104,1.7107608418
O, -2.8758263884,2.8207644389,0.2794899135
H, -3.5582245763,2.1299790492,0.2396448634

Zero-point correction=	0.647550 (Hartree/Particle)
Thermal correction to Energy=	0.689648
Thermal correction to Enthalpy=	0.690593
Thermal correction to Gibbs Free Energy=	0.568945
Sum of electronic and zero-point Energies=	-2375.977989
Sum of electronic and thermal Energies=	-2375.935890
Sum of electronic and thermal Enthalpies=	-2375.934946
Sum of electronic and thermal Free Energies=	-2376.056594