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SUPPORTING INFORMATION FOR

The mechanism of photocatalyzed imine conversion: a relayed process of sequential energy transfer, single electron transfer and proton transfer

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Part 1: Marcus theory

The SET processes from an acceptor oxidant and electron donor were calculated using Marcus Theory at 25 °C. The Gibbs free energy of activation of the SET is calculated using Marcus Theory and is shown below as an example (1). The same steps are taken to calculate the SET barrier for other substrates.

$$^3Ir(III) + Sub \rightarrow Ir(II)^{\cdot+} + Sub^{\cdot-} \quad (5)$$

The activation Gibbs free energy is therefore given by

$$\Delta G^{\neq} = \frac{(\Delta G + \lambda)^2}{4\lambda} \quad (6)$$

Here, λ is the reaction of internal reorganization energy, which calculated as

$$\lambda = \lambda_1 + \lambda_2 \quad (7)$$

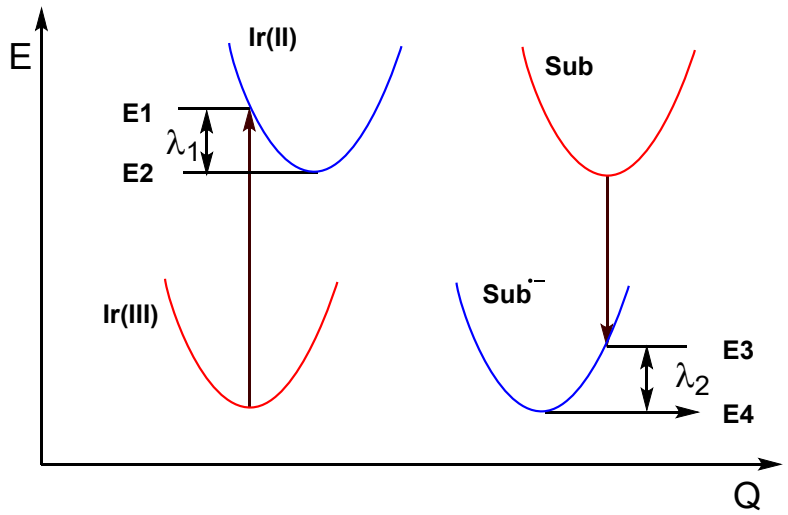


Figure S1. Four-point model of internal reorganization energy

Then, λ_1 is the reorganization energy of photosensitizer **Ir(III)***, and λ_2 is the reorganization energy of substrate **M1**.

$$\lambda_1 = E1 - E2 \quad (8)$$

$$\lambda_2 = E3 - E4 \quad (9)$$

Part 2: Details of the PCET process

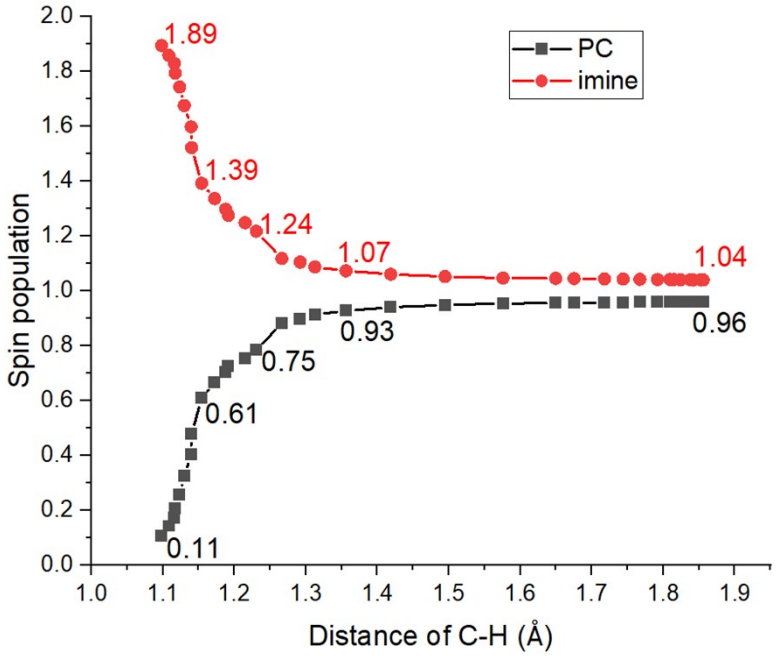


Figure S2. Fragment spin density as a function of C-H bond length (x-axis represents C-H bond length in Å, and y-axis represents the value of spin density).

We performed an IRC analysis on the key transition state TSpcet, as shown in Figure S2. We found that with an elongation of the C-H bond, the spin density on the photosensitizer gradually increases from 0.11 to 0.96, while the spin density on the iminium group gradually decreases from 1.89 to 1.04. This indicates that as the C-H bond breaks and the N-H bond forms, some electrons are transferred from the iminium group to the photosensitizer. These data suggest that TSpcet is a proton-coupled electron transfer process (PCET).

Part 3: Redox potentials

From the principles of chemical thermodynamics, we can easily derive the calculation formula for the half-cell potential of a battery like eq. (1). In this paper, the Gibbs free energy change in eq. (2) is used to calculate the redox potentials. The calculation based on eq. (3) yields the absolute electrode potential, which cannot be directly measured experimentally. However, by using eq. (4), it can be converted to the relative electrode potential, which is the experimentally measurable electrode potential (4.429 V vs SCE).[1]

$$A_{s}^{1M} \rightarrow A_{s}^{+,1M} + e_{gas}^{-,1atm} \quad (1)$$

$$\Delta G_{OX}^{\circ} = G^{\circ}\left(A_{s}^{+,1M}\right) - G^{\circ}\left(A_{s}^{1M}\right) \quad (2)$$

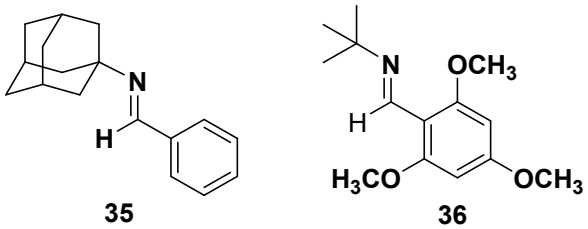
$$E_{OX}^{\circ,abs} = \frac{\Delta G_{OX}^{\circ}}{nF} \quad (3)$$

$$E_{OX}^{\circ,SCE} = E_{OX}^{\circ,abs} - 4.429 \quad (4)$$

From our results in Table S1, the largest derivation of calculated redox potential is about 200 mV compared to experimental value, indicating our results are consistent to experiments. It could be found that, the redox potential of triplet state is quite different to ground state, indicating the nature of redox pair could be change.

Table S1. The redox potentials of substrate and photocatalyst at ground state and triplet state, in V vs SCE. Compound 35 and 36 are shown in Scheme S1.

Redox pair	Redox potential	
	calculated	experimental
35 → $35^{\bullet+}$	1.707	1.861
36 → $36^{\bullet+}$	1.200	1.401
^{3}35 → $35^{\bullet+}$	-0.429	
^{3}36 → $36^{\bullet+}$	-0.870	
R1 → $R1^{\bullet+}$	1.174	
^{3}R1 → $R1^{\bullet+}$	-0.840	
$Ir^{\bullet-}$ → Ir	1.429	
$Ir^{\bullet-}$ → ^{3}Ir	-1.375	-1.21



Scheme S1. The species of 35 and 36 in Ttable S1.

Reference

1. Isse, A. A.; Gennaro, A., Absolute Potential of the Standard Hydrogen Electrode and the Problem of Interconversion of Potentials in Different Solvents. *J. Phys. Chem. B* **2010**, 114 (23), 7894-7899

Part 4: Energies, cartesian coordinates, and vibrational frequencies

R1

Zero-point correction= 0.446317
Thermal correction to Energy= 0.470334
Thermal correction to Enthalpy= 0.471278
Thermal correction to Gibbs Free Energy= 0.393739
Sum of electronic and zero-point Energies= -981.515068
Sum of electronic and thermal Energies= -981.491051
Sum of electronic and thermal Enthalpies= -981.490107
Sum of electronic and thermal Free Energies= -981.567646

Cartesian coordinates

C	2.389957	0.483742	-0.663610
C	2.875560	0.065777	-2.054588
H	2.817167	-1.025017	-2.176932
H	2.231041	0.527254	-2.818797
H	3.908294	0.392135	-2.241408
C	2.523306	2.001620	-0.523959
H	1.893992	2.519185	-1.265225
H	2.231004	2.351968	0.477817
H	3.558218	2.319471	-0.695742
C	4.634601	-0.433486	0.621678
N	1.014672	-0.018249	-0.581796
C	0.053066	0.750430	-0.256419
H	0.209392	1.819856	-0.049056
C	-1.351051	0.354036	-0.122159
C	-1.829118	-0.977905	-0.157189
C	-2.313024	1.380898	0.079034
C	-3.192078	-1.269447	0.002173
C	-3.667353	1.101700	0.235375
C	-4.100812	-0.227909	0.195661
H	-3.534648	-2.299790	-0.025436
H	-4.411124	1.881410	0.385434
O	-1.834842	2.639349	0.104069
O	-0.924407	-1.947441	-0.336206
O	-5.422244	-0.414628	0.353813
C	-1.331773	-3.290906	-0.343545
H	-0.422998	-3.886985	-0.491900
H	-1.799302	-3.583004	0.612008
H	-2.035246	-3.502144	-1.166541
C	-2.716822	3.711544	0.321085

H	-3.225509	3.628716	1.295970
H	-2.106222	4.622561	0.311963
H	-3.476199	3.780109	-0.475515
C	-5.938024	-1.722785	0.333351
H	-5.514873	-2.339171	1.144141
H	-7.021029	-1.633819	0.481495
H	-5.748222	-2.220121	-0.632594
C	3.101855	-0.266601	0.493206
H	2.668326	-1.280377	0.499741
H	2.737084	0.211352	1.419580
C	4.877035	-0.966112	2.040923
H	5.946774	-1.172229	2.205107
H	4.550980	-0.237611	2.800349
H	4.322144	-1.902435	2.212820
C	5.183535	-1.474177	-0.361387
H	4.633543	-2.424909	-0.275161
H	5.120993	-1.142962	-1.405994
H	6.244205	-1.679227	-0.143651
C	5.415377	0.873014	0.465356
H	5.377391	1.258642	-0.564302
H	5.031699	1.655766	1.138337
H	6.476947	0.710288	0.712733

Vibrational frequencies

-12.6596	24.3791	29.8198
37.3360	71.8542	77.3305
95.4061	112.7709	120.9365
160.7111	176.1811	181.4546
186.5643	204.3127	210.2048
224.1284	237.4194	249.4221
257.9835	271.3934	276.6655
280.8818	288.9618	291.2384
311.4378	318.9407	321.7856
334.9051	348.9653	369.3471

PC

Zero-point correction= 0.710086
Thermal correction to Energy= 0.768513
Thermal correction to Enthalpy= 0.769457
Thermal correction to Gibbs Free Energy= 0.611097
Sum of electronic and zero-point Energies= -3876.605238
Sum of electronic and thermal Energies= -3876.546811
Sum of electronic and thermal Enthalpies= -3876.545867

Sum of electronic and thermal Free Energies= -3876.704228

Cartesian coordinates

Ir	1.344447	-0.377678	-0.059043
C	-1.304130	-3.792665	-2.177827
C	-1.693861	-3.309650	-0.928511
C	-0.942561	-2.303658	-0.344343
C	0.581542	-2.287736	-2.126553
C	-0.168550	-3.276152	-2.778889
H	-1.882152	-4.572793	-2.676952
H	-1.228457	-1.876929	0.615313
H	0.156112	-3.644408	-3.748011
C	3.653556	-0.178071	-2.045332
C	2.435183	-0.766144	-1.692835
C	1.834592	-1.700076	-2.583427
C	2.480450	-1.990598	-3.794472
C	3.683328	-1.406131	-4.152864
C	4.248649	-0.504615	-3.256996
H	4.159106	0.539075	-1.396485
H	4.162860	-1.648987	-5.100689
N	0.157756	-1.811809	-0.921439
F	1.941982	-2.854501	-4.657575
F	5.406556	0.064157	-3.583457
C	-2.849651	-3.922126	-0.190472
F	-3.279206	-3.148296	0.801926
F	-2.486453	-5.095377	0.354781
F	-3.872317	-4.178873	-1.003639
C	-2.175253	0.612604	3.258379
C	-1.118060	-0.242751	3.602514
C	-0.091514	-0.471286	2.702906
C	-1.030439	0.973991	1.153849
C	-2.095542	1.235688	2.013329
H	-1.095062	-0.760912	4.562006
H	0.726369	-1.157484	2.933633
C	-1.697545	3.019162	-1.972936
C	-1.808547	2.531130	-0.671754
C	-0.919070	1.573015	-0.191216
C	0.230158	1.585915	-2.202436
C	-0.634821	2.522097	-2.741020
H	-2.618803	2.865919	-0.032084
H	1.066175	1.184291	-2.778867
H	-0.473099	2.849807	-3.768536
N	-0.056626	0.106500	1.495756

N	0.092332	1.117828	-0.955840
C	4.359874	-1.889276	2.488937
C	4.187598	-3.259708	2.572196
C	3.144221	-3.818761	1.840210
C	2.291624	-3.061102	1.048546
C	2.468179	-1.676223	0.970006
C	3.528048	-1.073388	1.706440
H	4.846557	-3.870880	3.188303
H	1.497972	-3.574623	0.503443
C	4.581956	2.563904	1.943921
C	4.603487	1.199765	2.171264
C	3.639668	0.371709	1.573939
C	2.662741	2.244383	0.553252
C	3.590495	3.101563	1.118927
H	5.334378	3.207429	2.404431
H	5.366212	0.760620	2.808277
H	1.875308	2.617107	-0.101057
F	2.964995	-5.134980	1.908265
F	5.360007	-1.355876	3.193811
N	2.687465	0.925285	0.770861
C	3.530005	4.578533	0.857976
F	4.684317	5.029459	0.358896
F	3.300322	5.260752	1.984228
F	2.563815	4.892270	-0.006877
C	-2.694253	4.003953	-2.568853
C	-3.725303	4.462119	-1.536991
H	-3.251390	4.984604	-0.691306
H	-4.427476	5.164333	-2.009889
H	-4.306787	3.615321	-1.145024
C	-1.941668	5.227984	-3.107804
H	-2.656652	5.940613	-3.546575
H	-1.395780	5.743548	-2.302585
H	-1.219239	4.958064	-3.892192
C	-3.429852	3.287247	-3.713154
H	-2.737726	2.968400	-4.507077
H	-3.957217	2.399312	-3.335122
H	-4.168133	3.968502	-4.163935
H	-2.898602	1.883657	1.675483
C	-3.362091	0.797757	4.194325
C	-4.052033	-0.567863	4.348749
H	-3.381121	-1.315530	4.797981
H	-4.931029	-0.468129	5.004148
H	-4.385914	-0.940792	3.370013

C	-2.860239	1.292852	5.557586
H	-2.352545	2.265168	5.463205
H	-3.712166	1.417455	6.243309
H	-2.159292	0.584539	6.023757
C	-4.374247	1.798953	3.637552
H	-3.929684	2.798100	3.508384
H	-4.780036	1.467771	2.671237
H	-5.213635	1.898365	4.341449
P	-4.782218	-0.033639	-0.502389
F	-3.160915	-0.237580	-0.564790
F	-4.783491	-0.583999	1.031033
F	-4.565690	1.494865	0.065909
F	-6.388129	0.180896	-0.434368
F	-4.758943	0.545716	-2.024633
F	-4.991453	-1.539466	-1.065499

Vibrational frequencies

7.6051	11.4505	14.9324
15.2070	18.9460	23.3246
27.6772	30.0053	33.3475
34.5853	39.7170	50.9740
54.9899	56.3133	62.0682
63.9171	65.8914	68.1606
69.4367	72.9955	73.8454
76.9431	80.4372	84.7619
105.1284	125.5843	133.4863
140.5978	143.1985	145.7607

PC*

Zero-point correction= 0.710301
Thermal correction to Energy= 0.769137
Thermal correction to Enthalpy= 0.770081
Thermal correction to Gibbs Free Energy= 0.608480
Sum of electronic and zero-point Energies= -3876.498189
Sum of electronic and thermal Energies= -3876.439354
Sum of electronic and thermal Enthalpies= -3876.438410
Sum of electronic and thermal Free Energies= -3876.600011

Cartesian coordinates

Ir	1.403182	-0.374013	-0.052116
C	-0.836213	-4.322542	-1.663262
C	-1.423258	-3.588958	-0.606364
C	-0.806125	-2.430023	-0.175842

C	0.920357	-2.665298	-1.771162
C	0.323459	-3.852850	-2.239696
H	-1.295162	-5.245727	-2.020924
H	-1.233920	-1.839103	0.633460
H	0.788484	-4.393732	-3.060244
C	3.604787	-0.067667	-2.088760
C	2.499982	-0.801571	-1.623659
C	2.095533	-2.018706	-2.286466
C	2.885122	-2.451708	-3.369317
C	3.971322	-1.731306	-3.825513
C	4.315577	-0.535171	-3.175556
H	3.922217	0.856504	-1.604716
H	4.549386	-2.092224	-4.677018
N	0.336473	-1.989307	-0.713583
F	2.590133	-3.588649	-4.000608
F	5.363874	0.145686	-3.632277
C	-2.659843	-4.098531	0.063196
F	-3.097602	-3.280733	1.017998
F	-2.432082	-5.293316	0.639287
F	-3.652529	-4.289433	-0.810401
C	-2.093056	1.097104	3.180930
C	-1.030658	0.285982	3.605586
C	-0.049064	-0.095865	2.708927
C	-1.064826	1.074200	0.987873
C	-2.071315	1.505830	1.848244
H	-0.963916	-0.074236	4.632643
H	0.778908	-0.738910	3.013035
C	-1.947221	2.446503	-2.437915
C	-2.006136	2.190297	-1.068279
C	-1.033730	1.410253	-0.447718
C	0.070776	1.122690	-2.462028
C	-0.865242	1.888776	-3.133489
H	-2.839487	2.562034	-0.480552
H	0.920048	0.677591	-2.983529
H	-0.740991	2.037554	-4.206755
N	-0.074031	0.275054	1.422163
N	-0.007671	0.890093	-1.145710
C	4.450313	-1.313574	2.669574
C	4.297946	-2.651013	2.987545
C	3.235640	-3.359481	2.416086
C	2.346419	-2.763448	1.539459
C	2.505832	-1.407104	1.218045
C	3.568645	-0.639873	1.806273

H	4.995437	-3.136638	3.670694
H	1.543077	-3.364097	1.111428
C	4.382317	3.050296	1.569312
C	4.522162	1.726805	1.931750
C	3.612063	0.760670	1.463298
C	2.452849	2.435801	0.273538
C	3.310366	3.418917	0.726171
H	5.088804	3.798639	1.932364
H	5.332653	1.419471	2.587986
H	1.628274	2.676902	-0.398117
F	3.093985	-4.644159	2.731536
F	5.475719	-0.663858	3.221750
N	2.600232	1.149548	0.609033
C	3.115145	4.846663	0.328019
F	4.203794	5.342399	-0.273966
F	2.881368	5.625912	1.392235
F	2.087685	4.999931	-0.512004
C	-2.995500	3.276506	-3.165592
C	-4.085311	3.771709	-2.214648
H	-3.676658	4.437535	-1.438560
H	-4.831898	4.345857	-2.782550
H	-4.599827	2.934533	-1.722557
C	-2.301816	4.484364	-3.812889
H	-3.045151	5.098944	-4.343318
H	-1.815006	5.115774	-3.053731
H	-1.538789	4.178831	-4.544357
C	-3.644553	2.400706	-4.248911
H	-2.909064	2.045879	-4.986229
H	-4.133726	1.528281	-3.794027
H	-4.404182	2.985371	-4.790279
H	-2.874931	2.118903	1.453443
C	-3.236864	1.442611	4.123763
C	-3.997466	0.136062	4.409394
H	-3.352524	-0.611609	4.895387
H	-4.845529	0.339687	5.081576
H	-4.388737	-0.294875	3.475980
C	-2.677465	2.026332	5.427386
H	-2.108003	2.949014	5.236491
H	-3.506089	2.272202	6.108571
H	-2.018449	1.319154	5.952054
C	-4.205935	2.447109	3.499260
H	-3.704314	3.395168	3.249872
H	-4.674440	2.047706	2.588405

H	-5.007830	2.673006	4.217251
P	-4.882225	-0.233297	-0.319566
F	-3.281969	-0.505347	-0.114597
F	-5.159518	-0.758925	1.195029
F	-4.691041	1.294483	0.262117
F	-6.465117	0.056600	-0.521101
F	-4.581377	0.325132	-1.822769
F	-5.064812	-1.733685	-0.899942

Vibrational frequencies

0.9688	14.5771	16.6055
20.4915	22.8049	23.8225
27.9716	29.9308	35.0006
37.1621	38.5060	45.0591
51.3857	53.4583	57.9849
61.6973	64.8255	65.7202
67.3583	71.1184	74.7339
77.0254	79.2957	84.1929
105.2411	124.7025	129.6249
139.7315	142.5343	143.2056

PC$^{\bullet-}$

Zero-point correction= 0.706721
Thermal correction to Energy= 0.765322
Thermal correction to Enthalpy= 0.766266
Thermal correction to Gibbs Free Energy= 0.606451
Sum of electronic and zero-point Energies= -3876.707917
Sum of electronic and thermal Energies= -3876.649316
Sum of electronic and thermal Enthalpies= -3876.648372
Sum of electronic and thermal Free Energies= -3876.808188

Cartesian coordinates

Ir	1.438108	-0.367704	-0.086427
C	-1.412858	-3.527112	-2.318505
C	-1.748243	-3.093912	-1.034445
C	-0.927519	-2.168403	-0.411665
C	0.551990	-2.126969	-2.232998
C	-0.265519	-3.037876	-2.919196
H	-2.045636	-4.243516	-2.846034
H	-1.161259	-1.774945	0.576825
H	0.013574	-3.361970	-3.917892
C	3.699201	-0.129256	-2.143765
C	2.469207	-0.690204	-1.777783

C	1.813327	-1.561247	-2.696425
C	2.413789	-1.813987	-3.938399
C	3.625070	-1.253298	-4.307084
C	4.246663	-0.414839	-3.386121
H	4.245844	0.539370	-1.475620
H	4.067880	-1.465524	-5.279777
N	0.187506	-1.708959	-0.988120
F	1.822364	-2.619733	-4.827081
F	5.415790	0.131077	-3.723917
C	-2.926949	-3.674386	-0.310307
F	-3.290255	-2.941600	0.737414
F	-2.635220	-4.903862	0.153336
F	-3.979832	-3.814378	-1.115489
C	-2.069335	0.324841	3.296557
C	-0.945286	-0.499464	3.614998
C	0.073995	-0.629819	2.698136
C	-0.947233	0.856574	1.191712
C	-2.037872	0.993402	2.094102
H	-0.886932	-1.052673	4.552681
H	0.926492	-1.286098	2.894842
C	-1.691249	3.056167	-1.775940
C	-1.810235	2.465495	-0.538473
C	-0.865115	1.513020	-0.070208
C	0.321733	1.748910	-2.082143
C	-0.567963	2.678800	-2.572747
H	-2.659054	2.697886	0.098853
H	1.185897	1.432571	-2.672695
H	-0.402721	3.095675	-3.566566
N	0.087550	-0.001103	1.512650
N	0.201428	1.173515	-0.876174
C	4.496892	-2.018713	2.327493
C	4.325367	-3.391810	2.343590
C	3.267251	-3.911645	1.601645
C	2.402186	-3.114264	0.867378
C	2.574698	-1.724300	0.856592
C	3.652394	-1.163434	1.603821
H	4.994308	-4.034195	2.915518
H	1.595407	-3.595312	0.310791
C	4.707742	2.460568	2.006908
C	4.736272	1.086717	2.164355
C	3.764700	0.286660	1.540650
C	2.766687	2.205478	0.629453
C	3.700342	3.035585	1.226197

H	5.464753	3.083199	2.488227
H	5.508345	0.617886	2.768283
H	1.960195	2.597656	0.009236
F	3.090250	-5.232940	1.606043
F	5.513216	-1.523105	3.042045
N	2.801588	0.877093	0.777490
C	3.629969	4.522707	1.047197
F	4.777259	5.007867	0.557793
F	3.415554	5.145739	2.211805
F	2.652406	4.881830	0.214245
C	-2.716308	4.039691	-2.329424
C	-3.789075	4.392120	-1.298591
H	-3.351064	4.873689	-0.410166
H	-4.509296	5.097537	-1.741031
H	-4.342239	3.501451	-0.969618
C	-2.009875	5.330779	-2.765581
H	-2.743290	6.045512	-3.171697
H	-1.504075	5.809255	-1.912129
H	-1.256353	5.147267	-3.545794
C	-3.400301	3.384745	-3.540375
H	-2.672012	3.122149	-4.322616
H	-3.923802	2.467921	-3.232012
H	-4.136954	4.075345	-3.982180
H	-2.886442	1.596311	1.780489
C	-3.260339	0.381100	4.246052
C	-3.900402	-1.016355	4.288179
H	-3.185077	-1.778398	4.633364
H	-4.761220	-1.023143	4.976459
H	-4.254166	-1.302750	3.286767
C	-2.783650	0.777146	5.650161
H	-2.315673	1.774138	5.639377
H	-3.637445	0.808935	6.345648
H	-2.050832	0.063800	6.055489
C	-4.316811	1.385120	3.784081
H	-3.904865	2.404796	3.724733
H	-4.723636	1.117707	2.799332
H	-5.150173	1.401682	4.503516
P	-5.147605	0.059054	-0.452632
F	-3.563317	-0.288920	-0.582060
F	-5.196784	-0.662299	1.008273
F	-4.782897	1.483945	0.274877
F	-6.730155	0.417788	-0.324372
F	-5.102909	0.800040	-1.906598

F -5.522053 -1.347625 -1.173607

Vibrational frequencies

1.7938 12.8592 15.6998

17.2237 20.8216 25.5874

30.3113 33.4308 35.4160

35.8711 41.7681 48.2760

51.1204 58.4084 62.4890

64.2562 66.4593 72.3533

73.2966 74.7429 76.7279

78.6899 80.7465 86.8160

103.3706 121.1562 136.0840

140.4963 144.3207 148.8096

A1

Zero-point correction= 0.634412

Thermal correction to Energy= 0.671427

Thermal correction to Enthalpy= 0.672371

Thermal correction to Gibbs Free Energy= 0.562183

Sum of electronic and zero-point Energies= -1343.174969

Sum of electronic and thermal Energies= -1343.137955

Sum of electronic and thermal Enthalpies= -1343.137011

Sum of electronic and thermal Free Energies= -1343.247199

Cartesian coordinates

C 2.405456 1.039262 1.051871

C 2.886722 2.093491 2.048724

H 2.922255 3.087058 1.577382

H 2.173314 2.148672 2.886864

H 3.878677 1.859449 2.463359

C 2.390939 -0.324437 1.747636

H 1.557973 -0.361406 2.465716

H 2.252097 -1.151769 1.039157

H 3.325551 -0.501817 2.298305

N 1.048921 1.510727 0.634450

C 0.083689 0.738688 0.325485

C -0.108483 -0.692437 0.250937

C -0.780203 -1.404951 1.280576

C 0.055042 -1.389829 -0.975692

C -1.274870 -2.694992 1.098007

C -0.445757 -2.677783 -1.178204

C -1.117257 -3.327744 -0.139753

H -1.788500 -3.231964 1.896035

H	-0.320476	-3.200393	-2.127019
O	0.711818	-0.682331	-1.940442
O	-0.912043	-0.710587	2.446372
O	-1.625424	-4.592847	-0.335518
C	-1.594484	-1.311494	3.507593
H	-1.602385	-0.588194	4.333656
H	-2.638349	-1.559312	3.242070
H	-1.096016	-2.235832	3.850724
C	0.862565	-1.255290	-3.205664
H	-0.112339	-1.473818	-3.678343
H	1.401619	-0.525676	-3.824327
H	1.448963	-2.190815	-3.169532
C	-0.741199	-5.630488	0.009842
H	-0.462655	-5.591734	1.078850
H	-1.250055	-6.585054	-0.188181
H	0.187400	-5.591741	-0.588578
C	3.196875	1.034023	-0.273235
H	2.916580	1.969727	-0.789661
H	2.742496	0.229097	-0.874612
C	5.304218	-0.269554	0.412382
H	5.231621	-0.102586	1.496788
H	4.776309	-1.207233	0.178794
H	6.370475	-0.412975	0.170868
C	5.027431	0.659017	-1.871827
H	4.619277	1.471251	-2.494973
H	6.112492	0.602331	-2.057533
H	4.573617	-0.285038	-2.213959
C	4.733579	0.904602	-0.385362
C	5.455779	2.192885	0.024338
H	5.055938	3.059911	-0.525789
H	5.358561	2.403597	1.097552
H	6.532264	2.118669	-0.202600
N	-3.188269	0.897724	-0.999146
C	-3.748235	1.907099	-0.331183
N	-3.183648	3.125089	-0.286540
N	-4.923899	1.712442	0.285657
H	-5.503040	0.913110	0.069801
C	-3.525318	-0.481722	-0.703078
H	-2.630476	-1.101313	-0.847996
H	-3.833947	-0.584298	0.344349
H	-4.328061	-0.854404	-1.362386
C	-2.262107	1.107066	-2.096608
H	-2.378008	2.121011	-2.496766

H	-1.224807	0.948966	-1.751837
H	-2.506661	0.389431	-2.893243
C	-1.740715	3.305102	-0.212209
H	-1.358996	3.828233	-1.103268
H	-1.517306	3.921910	0.672406
H	-1.220003	2.324533	-0.082813
C	-3.987769	4.301250	-0.024915
H	-3.561185	5.147579	-0.581751
H	-5.019951	4.150142	-0.365793
H	-3.993220	4.568943	1.046219
H	-5.212983	2.307408	1.049843

Vibrational frequencies

7.0306	13.3267	16.2875
22.1140	27.3717	34.0197
41.7318	46.7498	51.7369
63.4902	80.9794	89.6504
102.0721	121.2043	125.0161
132.8003	143.4944	155.3449
161.5553	168.8702	186.0421
197.6227	206.5622	215.2721
217.2929	230.9295	237.2941
242.8529	243.9725	247.5875

^{3}M1

Zero-point correction= 1.154957
Thermal correction to Energy= 1.240151
Thermal correction to Enthalpy= 1.241095
Thermal correction to Gibbs Free Energy= 1.028327
Sum of electronic and zero-point Energies= -4858.060199
Sum of electronic and thermal Energies= -4857.975005
Sum of electronic and thermal Enthalpies= -4857.974061
Sum of electronic and thermal Free Energies= -4858.186829

Cartesian coordinates

Ir	-2.532149	-0.338512	-0.202677
C	-3.329796	4.411615	0.058827
C	-2.589103	3.801306	1.068752
C	-2.321981	2.446963	0.967229
C	-3.607579	2.255400	-0.980602
C	-3.837257	3.636745	-0.971118
H	-3.526065	5.485028	0.083608
H	-1.707774	1.943678	1.712102

H	-4.438190	4.088588	-1.755186
C	-4.435368	-1.084181	-2.448922
C	-3.882444	-0.083691	-1.645495
C	-4.183771	1.283320	-1.906125
C	-5.029042	1.582630	-2.982962
C	-5.579026	0.598353	-3.789697
C	-5.271167	-0.726510	-3.498976
H	-4.224562	-2.140973	-2.279899
H	-6.230755	0.862518	-4.622291
N	-2.817014	1.700702	-0.022916
F	-5.333295	2.846590	-3.273139
F	-5.796148	-1.677991	-4.262764
C	-2.156319	4.580532	2.278101
F	-1.393680	3.854488	3.096105
F	-3.234944	4.961003	2.983647
F	-1.495815	5.689360	1.963628
C	1.284130	0.665694	2.722062
C	0.156738	0.043291	3.278983
C	-0.854247	-0.426958	2.455664
C	0.327471	0.158176	0.557191
C	1.375600	0.648353	1.330352
H	0.021684	-0.029224	4.358532
H	-1.771069	-0.851845	2.870510
C	1.428650	0.681722	-3.024550
C	1.490999	0.506646	-1.643651
C	0.336642	0.239622	-0.913026
C	-0.931463	0.210045	-2.845868
C	0.172438	0.513879	-3.622334
H	2.436320	0.591410	-1.116375
H	-1.916213	0.069171	-3.294877
H	0.036008	0.624532	-4.698651
N	-0.797830	-0.324636	1.121531
N	-0.855076	0.078652	-1.516506
C	-5.062864	-2.701247	2.207631
C	-5.755210	-1.827505	3.004526
C	-5.523151	-0.438556	2.869235
C	-4.617205	0.063818	1.957421
C	-3.890115	-0.813793	1.141203
C	-4.107469	-2.260717	1.248780
H	-6.476028	-2.201170	3.733196
H	-4.488938	1.144753	1.890350
C	-2.540243	-5.155799	-0.587352
C	-3.384929	-4.496732	0.262983

C	-3.345200	-3.078589	0.387666
C	-1.624623	-3.002361	-1.246486
C	-1.615359	-4.384218	-1.364995
H	-2.574096	-6.241724	-0.680202
H	-4.101029	-5.052409	0.864253
H	-0.957709	-2.391146	-1.855298
F	-6.215338	0.381728	3.655933
F	-5.296995	-4.009013	2.353260
N	-2.435111	-2.351971	-0.419126
C	-0.623234	-5.060781	-2.243305
F	-1.186369	-6.007141	-3.002272
F	0.336675	-5.678751	-1.524317
F	0.002389	-4.205071	-3.061627
C	2.638831	1.073990	-3.859479
C	3.875802	1.282120	-2.988372
H	4.175579	0.360278	-2.467859
H	4.720237	1.597716	-3.617904
H	3.704145	2.064175	-2.234512
C	2.921637	-0.028365	-4.889018
H	3.784430	0.254465	-5.511496
H	3.159363	-0.981728	-4.392670
H	2.064965	-0.196520	-5.558731
C	2.315031	2.395835	-4.574612
H	1.470641	2.291022	-5.272201
H	2.065122	3.181081	-3.846074
H	3.189645	2.724331	-5.156955
H	2.222975	1.105991	0.828854
C	2.269465	1.448282	3.580400
C	1.526249	2.714749	4.042452
H	0.648692	2.466780	4.658707
H	2.203082	3.337247	4.648447
H	1.184467	3.302565	3.179485
C	2.714159	0.636338	4.799390
H	3.303918	-0.236063	4.492792
H	3.347885	1.263587	5.444467
H	1.865775	0.291971	5.408719
C	3.502789	1.868590	2.779492
H	4.024189	1.000944	2.349488
H	3.241832	2.555718	1.961030
H	4.206689	2.394957	3.440843
P	0.901863	4.187762	-0.551188
F	-0.080674	3.081253	-1.242624
F	0.434242	3.657792	0.924754

F	2.127917	3.099166	-0.532199
F	1.874751	5.279389	0.150974
F	1.379257	4.685580	-2.025563
F	-0.313534	5.264580	-0.567691
C	6.657946	-0.008776	0.179255
C	6.394228	1.479750	-0.058307
H	5.697748	1.626794	-0.893836
H	5.937669	1.918948	0.841828
H	7.322855	2.028920	-0.266901
C	7.654281	-0.157877	1.331722
H	7.226148	0.239001	2.265938
H	7.941227	-1.206351	1.503385
H	8.572221	0.404772	1.126640
C	8.262094	-0.312706	-2.024528
N	5.337621	-0.591880	0.447648
C	5.161163	-1.377966	1.432220
H	5.963748	-1.605082	2.151463
C	3.890958	-2.030044	1.762893
C	2.891220	-2.367660	0.825448
C	3.673373	-2.411055	3.110443
C	1.706840	-3.004565	1.222392
C	2.500540	-3.034304	3.519571
C	1.513366	-3.316590	2.569619
H	0.948360	-3.254358	0.485919
H	2.313754	-3.308960	4.555579
O	4.669134	-2.112173	3.970105
O	3.137190	-2.088667	-0.464856
O	0.403253	-3.905379	3.044328
C	2.369657	-2.718181	-1.458242
H	2.837793	-2.470305	-2.418531
H	2.355283	-3.812220	-1.328977
H	1.334348	-2.344916	-1.474764
C	4.605659	-2.594545	5.290587
H	4.517764	-3.693066	5.313125
H	5.542580	-2.295282	5.775447
H	3.760281	-2.153024	5.843715
C	-0.611280	-4.269071	2.141907
H	-0.251260	-4.993860	1.393387
H	-1.410231	-4.731582	2.733388
H	-1.018996	-3.389075	1.620403
C	7.120099	-0.775768	-1.088550
H	6.221649	-0.895063	-1.716452
H	7.364962	-1.793879	-0.737796

C	8.573208	-1.515216	-2.926630
H	9.338127	-1.255456	-3.675669
H	8.949652	-2.367192	-2.338272
H	7.672024	-1.849496	-3.465442
C	7.826004	0.843457	-2.931324
H	6.911553	0.582215	-3.486275
H	7.627085	1.767313	-2.372928
H	8.614024	1.065603	-3.668893
C	9.546833	0.075151	-1.290205
H	9.429776	1.003563	-0.711926
H	9.875249	-0.718836	-0.601527
H	10.358268	0.244927	-2.016239

Vibrational frequencies

11.4714	15.4416	17.8297
22.0915	23.2116	25.9571
27.7187	29.2152	30.3965
33.6166	35.3236	36.6354
38.4670	40.5916	41.8313
44.2140	46.2917	47.9418
51.6497	52.1412	56.1611
56.8383	65.0266	66.8361
69.3270	69.8881	73.9222
76.7036	78.8272	81.9003

^{3}B1

Zero-point correction= 1.155597

Thermal correction to Energy= 1.240287

Thermal correction to Enthalpy= 1.241231

Thermal correction to Gibbs Free Energy= 1.029696

Sum of electronic and zero-point Energies= -4858.053471

Sum of electronic and thermal Energies= -4857.968781

Sum of electronic and thermal Enthalpies= -4857.967837

Sum of electronic and thermal Free Energies= -4858.179372

Cartesian coordinates

Ir	-2.501197	-0.244333	-0.259580
C	-3.078523	4.495518	0.373165
C	-2.314227	3.778701	1.292072
C	-2.143966	2.418991	1.094235
C	-3.528223	2.432164	-0.798297
C	-3.684423	3.820580	-0.674008
H	-3.207017	5.574900	0.479389

H	-1.521512	1.828294	1.766608
H	-4.296532	4.359426	-1.392617
C	-4.544229	-0.732980	-2.494189
C	-3.906765	0.168643	-1.634319
C	-4.180040	1.560905	-1.769819
C	-5.056020	1.980553	-2.781174
C	-5.676961	1.093557	-3.644985
C	-5.405686	-0.259985	-3.474168
H	-4.377556	-1.811294	-2.430359
H	-6.352239	1.449944	-4.423113
N	-2.725404	1.769136	0.082970
F	-5.323777	3.277976	-2.949750
F	-5.998063	-1.128654	-4.292362
C	-1.756786	4.426411	2.522769
F	-0.763247	3.718246	3.054075
F	-2.708629	4.526384	3.468759
F	-1.320931	5.660819	2.292785
C	1.334932	0.388853	2.748669
C	0.174011	-0.287875	3.238345
C	-0.841082	-0.603536	2.362344
C	0.333857	0.256816	0.519370
C	1.400175	0.613595	1.391056
H	0.051855	-0.526695	4.295342
H	-1.764620	-1.069583	2.723026
C	1.344694	1.239682	-2.982230
C	1.414273	1.057625	-1.618438
C	0.315328	0.536378	-0.879823
C	-0.929589	0.428936	-2.869957
C	0.123712	0.884658	-3.628605
H	2.314037	1.333080	-1.070763
H	-1.890549	0.183693	-3.334366
H	-0.007471	0.993177	-4.706006
N	-0.802756	-0.332880	1.047467
N	-0.862808	0.259284	-1.540742
C	-5.101325	-2.793759	1.905101
C	-5.799619	-2.014352	2.808666
C	-5.542955	-0.644657	2.801115
C	-4.627980	-0.055645	1.941503
C	-3.915815	-0.847441	1.031757
C	-4.169443	-2.251524	1.006117
H	-6.517730	-2.459145	3.497741
H	-4.482026	1.025879	2.001322
C	-2.604641	-4.976942	-1.119562

C	-3.474699	-4.386260	-0.220867
C	-3.385018	-3.009483	0.046633
C	-1.637433	-2.821962	-1.508148
C	-1.650412	-4.182897	-1.762994
H	-2.662301	-6.049309	-1.318959
H	-4.223533	-4.983624	0.293099
H	-0.944574	-2.151182	-2.019442
F	-6.209543	0.119279	3.663090
F	-5.336751	-4.109133	1.920809
N	-2.473662	-2.253457	-0.633927
C	-0.606642	-4.793421	-2.646811
F	-1.110972	-5.741175	-3.433534
F	0.359248	-5.369372	-1.911323
F	-0.012644	-3.884375	-3.421691
C	2.484628	1.800573	-3.823361
C	3.716416	2.122695	-2.984735
H	4.146168	1.212344	-2.539406
H	4.491877	2.574976	-3.623456
H	3.485920	2.827401	-2.173300
C	2.871959	0.765226	-4.888252
H	3.725914	1.129230	-5.483357
H	3.165860	-0.189355	-4.420160
H	2.045888	0.554820	-5.584734
C	2.012439	3.093187	-4.503281
H	1.132404	2.924823	-5.142637
H	1.750724	3.845058	-3.744586
H	2.815501	3.502503	-5.138164
H	2.244039	1.154660	0.966357
C	2.366864	0.945206	3.726110
C	1.759098	2.191988	4.387746
H	0.802877	1.960276	4.883261
H	2.449851	2.590529	5.149770
H	1.578145	2.979171	3.641692
C	2.717414	-0.076923	4.811598
H	3.206839	-0.962650	4.382683
H	3.417484	0.373378	5.533606
H	1.836081	-0.413445	5.378095
C	3.656168	1.356798	3.018608
H	4.100235	0.507976	2.475566
H	3.490595	2.171567	2.298914
H	4.393287	1.708244	3.757840
P	1.782747	4.493665	0.186061
F	0.649741	3.344148	0.383546

F	1.938974	4.614934	1.802284
F	2.956221	3.339895	0.172763
F	2.920953	5.635800	-0.009270
F	1.646448	4.355569	-1.431715
F	0.624677	5.632451	0.192860
C	6.195441	-0.518329	-0.212179
C	5.690877	0.921105	-0.080338
H	4.626053	0.982555	-0.347350
H	5.805537	1.276290	0.953710
H	6.253104	1.590523	-0.741523
C	7.586224	-0.675786	0.424850
H	7.553418	-0.387171	1.485719
H	7.955740	-1.707023	0.340880
H	8.284416	0.002878	-0.083174
C	7.093227	-0.742226	-2.767685
N	5.328712	-1.343462	0.570083
C	5.017756	-1.933653	1.644862
C	3.770314	-2.555884	1.917131
C	2.743619	-2.592692	0.937171
C	3.541716	-3.152855	3.190026
C	1.519881	-3.190956	1.214592
C	2.318790	-3.727841	3.476359
C	1.311032	-3.728922	2.493507
H	0.732198	-3.206625	0.466228
H	2.090104	-4.176544	4.441464
O	4.564114	-3.088811	4.044700
O	3.055350	-2.041060	-0.233788
O	0.164932	-4.287628	2.869768
C	2.222756	-2.258796	-1.359144
H	2.708104	-1.758131	-2.204931
H	2.123999	-3.335886	-1.564894
H	1.236237	-1.798696	-1.201611
C	4.415419	-3.622141	5.344968
H	4.201699	-4.701977	5.307616
H	5.369143	-3.457352	5.858643
H	3.611305	-3.104739	5.892848
C	-0.913196	-4.342948	1.962614
H	-0.663763	-4.962730	1.085649
H	-1.754606	-4.797674	2.498771
H	-1.199135	-3.332047	1.632053
C	6.075901	-1.080932	-1.653785
H	5.065536	-0.793044	-1.993318
H	6.051367	-2.180612	-1.568228

C	6.429920	-1.202476	-4.071697
H	7.114689	-1.064881	-4.923377
H	6.158587	-2.270040	-4.026783
H	5.513419	-0.627694	-4.279352
C	7.415109	0.746935	-2.894609
H	6.505723	1.352401	-3.028512
H	7.967031	1.137889	-2.025715
H	8.053314	0.911113	-3.777631
C	8.395983	-1.532745	-2.606416
H	8.999954	-1.199530	-1.751609
H	8.195089	-2.609468	-2.482542
H	9.019354	-1.411571	-3.506743
H	5.780897	-1.960902	2.448103

Vibrational frequencies

10.3362	10.9536	16.8314
19.5993	21.7891	22.7416
24.8505	27.7769	31.7278
34.1846	35.4044	36.4880
39.2576	45.5639	46.5718
48.7641	50.4268	53.3808
54.9465	56.5877	60.2641
63.5404	64.7181	72.1722
74.2835	75.9380	77.4544
78.8447	80.5643	82.2924

^{3}B2

Zero-point correction= 1.347626
Thermal correction to Energy= 1.444264
Thermal correction to Enthalpy= 1.445208
Thermal correction to Gibbs Free Energy= 1.207695
Sum of electronic and zero-point Energies= -5219.835460
Sum of electronic and thermal Energies= -5219.738821
Sum of electronic and thermal Enthalpies= -5219.737877
Sum of electronic and thermal Free Energies= -5219.975390

Cartesian coordinates

Ir	3.298709	-0.552633	-0.084442
C	4.399620	3.659008	-2.130870
C	3.267214	2.967792	-2.565419
C	2.957110	1.758601	-1.966946
C	4.852404	1.857233	-0.588776
C	5.190382	3.102993	-1.140533

H	4.663929	4.624290	-2.567280
H	2.072093	1.195404	-2.258243
H	6.080072	3.619698	-0.791834
C	5.774434	-0.958506	1.675868
C	5.074554	-0.162290	0.761113
C	5.612983	1.108330	0.404055
C	6.813552	1.525787	0.997189
C	7.502807	0.746002	1.910706
C	6.959859	-0.495308	2.228703
H	5.409706	-1.942054	1.978898
H	8.432967	1.096538	2.357030
N	3.722807	1.222237	-1.011687
F	7.342682	2.715800	0.695024
F	7.612463	-1.261119	3.103846
C	2.441135	3.488881	-3.703042
F	1.290543	2.831514	-3.834276
F	3.103243	3.354289	-4.866315
F	2.171603	4.786197	-3.568858
C	-1.090959	0.022784	-2.203420
C	-0.192946	-0.957713	-2.726978
C	0.985115	-1.215191	-2.062395
C	0.461392	0.285795	-0.334974
C	-0.754935	0.598971	-0.999169
H	-0.396120	-1.484001	-3.659244
H	1.714400	-1.919793	-2.471982
C	0.536539	2.287151	2.858990
C	0.084151	1.769062	1.666155
C	0.886461	0.895655	0.882189
C	2.606079	1.095373	2.469826
C	1.852796	1.921126	3.273388
H	-0.905384	2.024605	1.296524
H	3.625684	0.815770	2.749554
H	2.285629	2.292461	4.202628
N	1.339345	-0.609707	-0.916938
N	2.160493	0.586078	1.310821
C	4.751744	-4.053595	-1.969476
C	5.301677	-3.681142	-3.182688
C	5.288275	-2.324048	-3.499304
C	4.750513	-1.360958	-2.658601
C	4.188894	-1.740392	-1.432956
C	4.199092	-3.121960	-1.077302
H	5.723910	-4.423150	-3.859732
H	4.773371	-0.317542	-2.979143

C	2.863985	-4.841913	2.030901
C	3.514201	-4.698493	0.818297
C	3.592379	-3.436760	0.205099
C	2.428767	-2.487213	2.008110
C	2.294144	-3.715381	2.633165
H	2.796870	-5.822303	2.506513
H	3.961292	-5.559173	0.328358
H	2.034788	-1.569780	2.445989
F	5.815955	-1.949886	-4.664102
F	4.754200	-5.357206	-1.670009
N	3.056942	-2.351567	0.836452
C	1.499958	-3.838869	3.897695
F	2.114319	-4.609658	4.795862
F	0.301825	-4.399240	3.659998
F	1.270091	-2.651439	4.462945
C	-0.292959	3.220985	3.733303
C	-1.677031	3.478340	3.141375
H	-2.248326	2.544389	3.035517
H	-2.247852	4.145103	3.806230
H	-1.609841	3.949496	2.152514
C	-0.456418	2.591980	5.124642
H	-1.047224	3.256084	5.775631
H	-0.980917	1.625396	5.060548
H	0.512550	2.417566	5.615845
C	0.440281	4.565609	3.854947
H	1.442913	4.446862	4.292717
H	0.544693	5.029557	2.863856
H	-0.130254	5.251337	4.502010
H	-1.383972	1.374191	-0.569906
C	-2.289958	0.486445	-3.024739
C	-1.753355	1.375995	-4.159279
H	-1.019361	0.836100	-4.777407
H	-2.580604	1.697473	-4.813655
H	-1.268988	2.272917	-3.748380
C	-3.032524	-0.709970	-3.631272
H	-3.404561	-1.384570	-2.847890
H	-3.892298	-0.356193	-4.222080
H	-2.394230	-1.298379	-4.306542
C	-3.268855	1.308014	-2.184369
H	-3.633701	0.740087	-1.315456
H	-2.809955	2.234880	-1.816367
H	-4.134765	1.593511	-2.801465
P	-0.706788	4.742102	-0.919682

F	0.432535	3.585682	-1.045059
F	-1.274792	4.348233	-2.396896
F	-1.741096	3.656216	-0.246736
F	-1.854428	5.887724	-0.787429
F	-0.155719	5.123860	0.567110
F	0.305740	5.824302	-1.581312
C	-5.500542	1.044887	1.872700
C	-5.264482	2.390708	1.177719
H	-4.202470	2.672241	1.216284
H	-5.549309	2.311302	0.117657
H	-5.859585	3.192392	1.629442
C	-6.977098	0.668036	1.805987
H	-7.304519	0.589334	0.760678
H	-7.164180	-0.296674	2.300271
H	-7.594652	1.437046	2.288938
C	-5.513092	1.742436	4.521493
N	-4.668316	0.093281	1.161127
C	-4.803856	-1.000242	0.603639
C	-3.757432	-1.907964	0.175059
C	-2.488917	-1.932298	0.812301
C	-3.991352	-2.849771	-0.854173
C	-1.494175	-2.829140	0.408470
C	-3.003355	-3.729400	-1.276318
C	-1.750141	-3.701898	-0.650092
H	-0.523614	-2.815723	0.894649
H	-3.153439	-4.431003	-2.093791
O	-5.217777	-2.815501	-1.416733
O	-2.306528	-1.078645	1.823096
O	-0.843632	-4.563546	-1.135063
C	-1.195615	-1.238461	2.672274
H	-1.303197	-0.489289	3.465315
H	-1.175536	-2.247382	3.114269
H	-0.252588	-1.042857	2.140362
C	-5.557542	-3.801196	-2.362478
H	-5.400383	-4.815073	-1.961334
H	-6.623166	-3.671936	-2.585460
H	-4.978178	-3.684359	-3.292783
C	0.436776	-4.598223	-0.554239
H	0.390122	-4.902963	0.504115
H	1.019391	-5.338957	-1.114751
H	0.935129	-3.618741	-0.628583
C	-4.918405	0.987077	3.310481
H	-3.863049	1.282804	3.206137

H	-4.890535	-0.081038	3.584544
C	-4.455953	1.630778	5.629556
H	-4.816399	2.093638	6.561825
H	-4.218201	0.576644	5.845603
H	-3.521116	2.134011	5.339798
C	-5.772691	3.226779	4.257269
H	-4.883674	3.726485	3.843049
H	-6.610003	3.383324	3.561176
H	-6.035130	3.734555	5.199193
C	-6.797618	1.086214	5.040586
H	-7.641101	1.196627	4.346335
H	-6.645952	0.010067	5.221528
H	-7.097790	1.547327	5.995135
N	-9.530424	-2.141221	-1.899812
C	-8.322094	-1.601288	-1.653230
N	-7.668405	-0.938391	-2.619622
N	-7.774727	-1.732392	-0.448327
H	-8.352924	-1.954216	0.351276
C	-10.035614	-3.234129	-1.092953
H	-10.660638	-3.879811	-1.725324
H	-9.203862	-3.835694	-0.705986
H	-10.652625	-2.877620	-0.250269
C	-10.493074	-1.498950	-2.776765
H	-10.127545	-0.513958	-3.086570
H	-10.702826	-2.106064	-3.670691
H	-11.434653	-1.354669	-2.225024
C	-7.785665	-1.300404	-4.020490
H	-8.279724	-0.510803	-4.607010
H	-6.775722	-1.454229	-4.430217
H	-8.346051	-2.235363	-4.130024
C	-6.619134	0.011938	-2.304470
H	-6.628656	0.809311	-3.059979
H	-6.794788	0.465937	-1.322917
H	-5.630114	-0.467612	-2.300787
H	-6.763939	-1.628905	-0.284389

Vibrational frequencies

10.0484	12.4824	16.2961
18.2578	19.0548	21.0682
24.7642	26.5902	27.9425
29.9617	31.5823	32.7370
36.4706	37.3471	38.5705
42.2114	44.5800	46.7188

47.7633 49.6464 51.6392
52.6771 58.0705 59.1118
62.2832 65.9676 66.9632
71.6748 74.6753 76.4882

TS1

Zero-point correction= 1.343426
Thermal correction to Energy= 1.439352
Thermal correction to Enthalpy= 1.440296
Thermal correction to Gibbs Free Energy= 1.201823
Sum of electronic and zero-point Energies= -5219.821746
Sum of electronic and thermal Energies= -5219.725820
Sum of electronic and thermal Enthalpies= -5219.724876
Sum of electronic and thermal Free Energies= -5219.963349

Cartesian coordinates

Ir	3.237449	-0.589922	-0.062765
C	4.499018	3.494598	-2.269643
C	3.334943	2.837732	-2.670058
C	2.980914	1.662144	-2.029255
C	4.888301	1.730902	-0.667172
C	5.275236	2.940272	-1.264681
H	4.800575	4.432272	-2.740004
H	2.069528	1.128528	-2.293300
H	6.186981	3.430239	-0.940483
C	5.693325	-1.023405	1.717601
C	5.027861	-0.237100	0.769437
C	5.621091	0.991263	0.353983
C	6.841477	1.379411	0.925389
C	7.497694	0.609800	1.871355
C	6.900173	-0.590355	2.245411
H	5.284760	-1.974514	2.063103
H	8.446044	0.937254	2.299965
N	3.730345	1.127621	-1.061125
F	7.423204	2.527326	0.569164
F	7.520259	-1.344090	3.154070
C	2.518657	3.360503	-3.814529
F	1.348418	2.732761	-3.929194
F	3.171838	3.189600	-4.976661
F	2.282815	4.666225	-3.698605
C	-1.142805	0.060543	-2.188103
C	-0.270774	-0.951361	-2.696210
C	0.903122	-1.224684	-2.029868

C	0.422213	0.322317	-0.328897
C	-0.790294	0.651192	-0.997160
H	-0.485697	-1.488796	-3.620147
H	1.615860	-1.953671	-2.428038
C	0.567093	2.396824	2.816345
C	0.094355	1.861208	1.640225
C	0.871028	0.953140	0.868843
C	2.612944	1.164485	2.430083
C	1.883133	2.019648	3.222981
H	-0.891850	2.134456	1.271402
H	3.631800	0.874816	2.703964
H	2.332814	2.405249	4.139339
N	1.275192	-0.606633	-0.895606
N	2.143206	0.634575	1.290645
C	4.628350	-4.212973	-1.753010
C	5.196904	-3.916537	-2.979522
C	5.208405	-2.578736	-3.367663
C	4.679956	-1.562136	-2.587248
C	4.100062	-1.866466	-1.347775
C	4.083249	-3.226779	-0.920109
H	5.613990	-4.699201	-3.610042
H	4.724907	-0.538117	-2.963006
C	2.651388	-4.762852	2.240165
C	3.337688	-4.692198	1.042272
C	3.450506	-3.463059	0.367613
C	2.253400	-2.407891	2.086483
C	2.077881	-3.601091	2.766406
H	2.555388	-5.718240	2.762945
H	3.783771	-5.581703	0.608025
H	1.856265	-1.465424	2.466781
F	5.753845	-2.275518	-4.546167
F	4.605918	-5.498035	-1.385154
N	2.921891	-2.339403	0.932251
C	1.234851	-3.649740	4.004397
F	1.791261	-4.403934	4.952891
F	0.027887	-4.178922	3.743891
F	1.023732	-2.434111	4.515027
C	-0.240750	3.356853	3.684587
C	-1.625455	3.626494	3.101304
H	-2.218243	2.701001	3.021141
H	-2.178012	4.315631	3.758515
H	-1.563063	4.076049	2.102368
C	-0.396010	2.747246	5.084138

H	-0.985098	3.417543	5.730114
H	-0.917788	1.778145	5.038543
H	0.575607	2.580893	5.571892
C	0.512306	4.691583	3.784748
H	1.515693	4.563011	4.216215
H	0.616356	5.145305	2.788017
H	-0.042571	5.391686	4.430329
H	-1.391078	1.459508	-0.589569
C	-2.326747	0.547105	-3.020992
C	-1.759565	1.413015	-4.160565
H	-1.041755	0.844297	-4.772476
H	-2.574152	1.754023	-4.818673
H	-1.246136	2.295856	-3.756689
C	-3.103505	-0.626525	-3.625112
H	-3.561222	-1.245578	-2.840569
H	-3.909241	-0.244549	-4.271206
H	-2.470747	-1.277160	-4.245880
C	-3.293745	1.394357	-2.194625
H	-3.674404	0.826987	-1.330140
H	-2.830310	2.316149	-1.820425
H	-4.151751	1.685246	-2.818454
P	-0.546481	4.765095	-1.002586
F	0.504185	3.531712	-1.165976
F	-1.181385	4.426215	-2.465325
F	-1.639646	3.747079	-0.311164
F	-1.606664	5.988650	-0.827307
F	0.069995	5.091816	0.470435
F	0.520905	5.778388	-1.683259
C	-5.542140	0.974192	2.020328
C	-5.188696	2.239899	1.229214
H	-4.098874	2.361097	1.149281
H	-5.605018	2.178434	0.213676
H	-5.602042	3.130320	1.716889
C	-7.059843	0.760309	2.061683
H	-7.454213	0.591707	1.049924
H	-7.317773	-0.111596	2.677857
H	-7.542574	1.650419	2.484365
C	-5.356472	1.744842	4.627099
N	-4.957775	-0.127127	1.309860
C	-5.055270	-1.026127	0.451801
H	-6.172575	-1.140302	-0.059744
C	-3.982456	-1.916628	0.070945
C	-2.740298	-1.887459	0.763012

C	-4.132116	-2.849641	-0.991510
C	-1.692481	-2.737329	0.411379
C	-3.088687	-3.689188	-1.350444
C	-1.872201	-3.624195	-0.655836
H	-0.747506	-2.686154	0.942849
H	-3.165245	-4.397220	-2.171743
O	-5.307611	-2.846178	-1.633043
O	-2.646746	-1.015781	1.765625
O	-0.923755	-4.457398	-1.086921
C	-1.533282	-1.054988	2.633682
H	-1.726516	-0.309141	3.414095
H	-1.429397	-2.049621	3.092577
H	-0.611197	-0.778686	2.102823
C	-5.507518	-3.752108	-2.695128
H	-5.389529	-4.795534	-2.356229
H	-6.533755	-3.598735	-3.039701
H	-4.808656	-3.555895	-3.523197
C	0.325270	-4.473186	-0.437488
H	0.223435	-4.783484	0.615132
H	0.947338	-5.202856	-0.968115
H	0.808469	-3.486394	-0.483694
C	-4.861054	0.920962	3.414385
H	-3.805035	1.172103	3.236822
H	-4.864249	-0.137309	3.724361
C	-4.243779	1.618773	5.679199
H	-4.532988	2.126653	6.612416
H	-4.039177	0.562028	5.918339
H	-3.306819	2.071966	5.323608
C	-5.561100	3.228384	4.322168
H	-4.669482	3.676047	3.859693
H	-6.420716	3.401656	3.655472
H	-5.764048	3.776323	5.256194
C	-6.637991	1.165512	5.238980
H	-7.516206	1.304526	4.598073
H	-6.528779	0.087601	5.442620
H	-6.852165	1.665092	6.196960
N	-8.769786	-2.498006	-2.144105
C	-8.038642	-1.428506	-1.695550
N	-7.695047	-0.483037	-2.619125
N	-7.668190	-1.274755	-0.455516
H	-8.121360	-1.932501	0.176840
C	-8.856924	-3.684053	-1.328569
H	-9.063555	-4.549277	-1.973899

H	-7.900981	-3.862677	-0.815965
H	-9.663486	-3.624557	-0.571802
C	-9.838207	-2.332842	-3.110136
H	-9.857210	-1.302422	-3.484254
H	-9.720705	-3.020708	-3.964211
H	-10.811365	-2.540826	-2.636060
C	-7.309732	-0.824600	-3.971400
H	-7.789505	-0.152042	-4.698609
H	-6.215049	-0.735841	-4.089868
H	-7.593112	-1.855330	-4.210598
C	-7.201094	0.792882	-2.157558
H	-7.377149	1.548279	-2.935658
H	-7.728961	1.092144	-1.243329
H	-6.117853	0.766908	-1.943208

Vibrational frequencies

-105.8470	2.3061	9.6562
12.8374	15.8974	16.9322
21.9526	23.2444	25.6614
28.7283	29.4084	31.2038
34.3878	35.1751	37.6021
38.0157	40.2866	42.1808
44.0632	46.6827	50.3365
52.1818	55.1439	58.6850
62.2145	62.7327	67.1755
68.8338	70.4891	73.9874

^{3}C1

Zero-point correction= 1.155804
Thermal correction to Energy= 1.240517
Thermal correction to Enthalpy= 1.241461
Thermal correction to Gibbs Free Energy= 1.030233
Sum of electronic and zero-point Energies= -4858.077703
Sum of electronic and thermal Energies= -4857.992990
Sum of electronic and thermal Enthalpies= -4857.992046
Sum of electronic and thermal Free Energies= -4858.203274

Cartesian coordinates

Ir	-2.076910	-0.742177	0.074103
C	-4.325808	3.513946	-0.273243
C	-3.386216	3.332804	0.739471
C	-2.718254	2.123470	0.815735
C	-3.974927	1.222672	-0.938558

C	-4.617546	2.455770	-1.115037
H	-4.840848	4.468724	-0.393233
H	-1.943288	1.965569	1.562724
H	-5.365600	2.564463	-1.894814
C	-3.872830	-2.412714	-1.756292
C	-3.563275	-1.167731	-1.197574
C	-4.287692	-0.021235	-1.631380
C	-5.263273	-0.174673	-2.627617
C	-5.561924	-1.402113	-3.195197
C	-4.854647	-2.505995	-2.733785
H	-3.363559	-3.330417	-1.460319
H	-6.325010	-1.490604	-3.967914
N	-2.997754	1.100751	0.002455
F	-5.949892	0.880066	-3.072063
F	-5.131850	-3.697738	-3.258617
C	-3.148459	4.408861	1.757701
F	-2.227823	4.051799	2.655897
F	-4.281674	4.657852	2.436003
F	-2.770774	5.562079	1.214927
C	1.240826	2.078790	2.297844
C	0.399398	1.283405	3.090058
C	-0.391798	0.304410	2.505077
C	0.470718	0.762236	0.415079
C	1.302058	1.745873	0.945194
H	0.308924	1.449214	4.164499
H	-1.090819	-0.287491	3.099742
C	1.180934	0.826770	-3.299414
C	1.376726	0.941693	-1.924545
C	0.392166	0.518411	-1.034506
C	-0.922517	-0.236512	-2.781146
C	-0.006394	0.208834	-3.717026
H	2.286767	1.381696	-1.525556
H	-1.850912	-0.725865	-3.082880
H	-0.236764	0.077320	-4.774955
N	-0.406646	0.084380	1.184705
N	-0.731514	-0.084223	-1.465614
C	-3.555739	-3.399461	3.009592
C	-4.386937	-2.678576	3.849108
C	-4.582532	-1.333005	3.551378
C	-3.978125	-0.706245	2.469862
C	-3.129967	-1.436328	1.630245
C	-2.921740	-2.819250	1.901445
H	-4.864814	-3.150782	4.706957

H	-4.185185	0.352425	2.304203
C	-1.088693	-5.426823	-0.149673
C	-1.873640	-4.902812	0.861164
C	-2.053830	-3.515086	0.964703
C	-0.656391	-3.191342	-0.883392
C	-0.453804	-4.552773	-1.035092
H	-0.974416	-6.507178	-0.255096
H	-2.380195	-5.560974	1.561926
H	-0.208215	-2.475821	-1.570693
F	-5.383598	-0.625258	4.344643
F	-3.361745	-4.688881	3.297541
N	-1.445165	-2.688869	0.068919
C	0.439985	-5.056191	-2.129226
F	-0.009425	-6.197460	-2.646996
F	1.686140	-5.297375	-1.678966
F	0.558983	-4.169289	-3.120162
C	2.157217	1.395544	-4.319604
C	3.364759	2.037599	-3.639730
H	3.923794	1.312757	-3.031393
H	4.051009	2.434992	-4.402028
H	3.059164	2.870402	-2.989335
C	2.635212	0.277935	-5.256250
H	3.320648	0.691386	-6.012000
H	3.173848	-0.504079	-4.699906
H	1.799493	-0.198996	-5.789587
C	1.415071	2.474622	-5.125365
H	0.570258	2.052409	-5.689845
H	1.024873	3.260285	-4.461751
H	2.104688	2.936116	-5.849248
H	1.926343	2.316315	0.264992
C	1.952616	3.305383	2.860602
C	0.868221	4.333976	3.224003
H	0.175997	3.944421	3.985416
H	1.343254	5.241293	3.629114
H	0.283051	4.608674	2.336690
C	2.749878	2.948967	4.119872
H	3.531882	2.207951	3.907660
H	3.225543	3.856556	4.521306
H	2.105062	2.538008	4.910937
C	2.882851	3.940720	1.824855
H	3.650730	3.238254	1.468563
H	2.319580	4.302453	0.952127
H	3.393856	4.804632	2.275064

P	-0.359870	4.458742	-1.427263
F	-0.502897	4.108237	0.164348
F	0.267633	5.907719	-1.048133
F	1.150253	3.818693	-1.419809
F	-0.200064	4.789137	-3.014265
F	-0.985053	2.997415	-1.793617
F	-1.853607	5.097068	-1.435786
C	6.221093	0.891134	0.006119
C	6.372208	1.212774	-1.476234
H	5.917380	0.426653	-2.094613
H	5.863633	2.162294	-1.696564
H	7.428843	1.313740	-1.758371
C	6.880356	2.004558	0.842471
H	6.393943	2.969802	0.636844
H	6.795929	1.790932	1.918366
H	7.944414	2.096724	0.591409
C	8.069974	-1.114046	-0.014926
N	4.793799	1.012070	0.316809
C	4.256993	0.457801	1.439181
C	3.448002	-0.693066	1.521680
C	3.136193	-1.532619	0.409838
C	2.879865	-1.056974	2.784294
C	2.322271	-2.651705	0.552047
C	2.052409	-2.163699	2.919492
C	1.776629	-2.956830	1.803524
H	2.110845	-3.300186	-0.293663
H	1.613242	-2.444902	3.874895
O	3.225366	-0.260882	3.814303
O	3.697502	-1.171893	-0.763428
O	0.947895	-4.027511	1.969758
C	3.493884	-1.973231	-1.897251
H	4.098317	-1.535030	-2.700823
H	3.822004	-3.012172	-1.727187
H	2.436143	-1.975875	-2.209593
C	2.756082	-0.566249	5.101838
H	3.098900	-1.561703	5.429712
H	3.167264	0.196179	5.774218
H	1.654801	-0.533347	5.152180
C	1.556323	-5.294313	1.846690
H	2.395694	-5.401189	2.555149
H	0.791025	-6.045151	2.083283
H	1.925653	-5.477908	0.824365
C	6.708903	-0.518141	0.412481

H	5.937453	-1.222770	0.065789
H	6.661743	-0.546575	1.514405
C	8.252052	-2.374708	0.841991
H	9.175586	-2.908146	0.566083
H	8.312668	-2.121737	1.912407
H	7.406901	-3.068945	0.707937
C	8.071013	-1.551096	-1.484521
H	7.214232	-2.210333	-1.698536
H	8.024867	-0.702771	-2.179270
H	8.991122	-2.112779	-1.712331
C	9.257203	-0.184881	0.244266
H	9.246873	0.698012	-0.412215
H	9.274648	0.165109	1.288328
H	10.202479	-0.718425	0.055053
H	4.388973	1.038614	2.359963

Vibrational frequencies

8.8018	15.2633	20.3658
21.3033	23.4817	24.7327
27.9374	30.3449	31.7332
32.9873	34.7310	37.0390
39.9185	42.7608	44.2163
46.7744	47.8010	51.0329
51.7313	52.6628	58.8324
59.9458	64.9957	71.0131
71.9447	74.8332	79.1502
79.5301	81.5063	82.7839

^{3}C2

Zero-point correction= 1.346543
Thermal correction to Energy= 1.443026
Thermal correction to Enthalpy= 1.443970
Thermal correction to Gibbs Free Energy= 1.205315
Sum of electronic and zero-point Energies= -5219.830975
Sum of electronic and thermal Energies= -5219.734492
Sum of electronic and thermal Enthalpies= -5219.733548
Sum of electronic and thermal Free Energies= -5219.972204

Cartesian coordinates

Ir	2.579129	-0.627902	-0.524626
C	4.625094	3.739351	-0.699884
C	3.400775	3.546530	-1.336433
C	2.802209	2.301571	-1.259604

C	4.626877	1.401590	-0.106857
C	5.237077	2.663384	-0.082673
H	5.106888	4.718694	-0.700287
H	1.824892	2.129955	-1.705695
H	6.203612	2.781801	0.398041
C	4.964393	-2.264378	0.478333
C	4.429304	-1.018093	0.133823
C	5.212046	0.150095	0.358109
C	6.478617	0.013752	0.945658
C	7.005893	-1.216193	1.302296
C	6.227555	-2.339717	1.050041
H	4.421887	-3.197686	0.323567
H	7.993078	-1.291449	1.757313
N	3.390362	1.261815	-0.660576
F	7.233257	1.088149	1.186714
F	6.717866	-3.533692	1.376733
C	2.777280	4.652279	-2.136178
F	1.598613	4.295183	-2.650116
F	3.572677	4.976825	-3.170010
F	2.601035	5.765023	-1.430124
C	-1.425472	2.066956	-1.315283
C	-0.862369	1.368032	-2.393034
C	0.128664	0.421982	-2.172099
C	0.004964	0.729581	0.112127
C	-1.004878	1.675998	-0.044436
H	-1.152928	1.584415	-3.421785
H	0.614980	-0.093726	-3.003136
C	0.610393	0.588000	3.843786
C	-0.052396	0.746780	2.628076
C	0.584457	0.426199	1.431152
C	2.452113	-0.318786	2.575521
C	1.894607	0.027534	3.793164
H	-1.062559	1.145770	2.589939
H	3.448832	-0.760768	2.511487
H	2.480040	-0.134641	4.699124
N	0.599981	0.146170	-0.949963
N	1.814312	-0.121081	1.416048
C	3.074363	-3.070223	-3.939185
C	3.528492	-2.265275	-4.969398
C	3.750667	-0.922245	-4.678901
C	3.528754	-0.377808	-3.421116
C	3.058961	-1.193141	-2.385642
C	2.835214	-2.575101	-2.649276

H	3.702431	-2.672266	-5.965056
H	3.730403	0.684783	-3.274540
C	1.961888	-5.370392	-0.242993
C	2.314700	-4.760121	-1.433032
C	2.378308	-3.360883	-1.513874
C	1.688975	-3.196280	0.716589
C	1.630822	-4.573220	0.854766
H	1.951097	-6.458771	-0.163172
H	2.577327	-5.358379	-2.301367
H	1.462512	-2.535575	1.551971
F	4.193327	-0.134311	-5.656303
F	2.855042	-4.357677	-4.217440
N	2.074154	-2.609391	-0.418840
C	1.219102	-5.174903	2.165616
F	1.853019	-6.322025	2.399628
F	-0.099931	-5.447081	2.197246
F	1.460655	-4.350368	3.187079
C	0.020759	1.046815	5.170300
C	-1.362988	1.664525	4.983116
H	-2.078317	0.943962	4.562600
H	-1.755639	1.994736	5.956180
H	-1.320137	2.538939	4.317300
C	-0.079451	-0.148583	6.127194
H	-0.488320	0.179243	7.095410
H	-0.744932	-0.925951	5.722355
H	0.902782	-0.606626	6.316888
C	0.958991	2.113285	5.758556
H	1.957107	1.704342	5.975737
H	1.077660	2.956751	5.062798
H	0.540958	2.493854	6.703526
H	-1.394368	2.168622	0.840771
C	-2.350579	3.261309	-1.531101
C	-1.506487	4.376526	-2.171585
H	-1.097137	4.066778	-3.144849
H	-2.135798	5.265555	-2.334929
H	-0.667241	4.653179	-1.520049
C	-3.506002	2.907980	-2.474737
H	-4.147548	2.116522	-2.064785
H	-4.126268	3.802072	-2.640086
H	-3.144563	2.574253	-3.458866
C	-2.912550	3.785992	-0.208047
H	-3.476135	3.015875	0.338243
H	-2.110525	4.153277	0.448902

H	-3.591819	4.627642	-0.408768
P	1.257130	4.373928	1.815011
F	0.851098	4.118635	0.251625
F	0.488622	5.804218	1.778357
F	-0.138142	3.650508	2.281168
F	1.646089	4.609022	3.379352
F	2.021427	2.932712	1.841686
F	2.638335	5.093965	1.354934
C	-5.181549	0.513095	2.320215
C	-4.831681	0.704641	3.791700
H	-4.211461	-0.123223	4.163535
H	-4.269097	1.641255	3.912575
H	-5.738104	0.767698	4.409119
C	-6.067592	1.683023	1.847481
H	-5.510395	2.627892	1.937727
H	-6.383286	1.545797	0.801856
H	-6.963439	1.759826	2.476773
C	-6.979050	-1.503935	2.714232
N	-3.938730	0.687400	1.562786
C	-3.789565	0.197559	0.301143
C	-3.027638	-0.921582	-0.091480
C	-2.372074	-1.799747	0.824333
C	-2.866691	-1.211256	-1.483897
C	-1.638974	-2.897262	0.383867
C	-2.121778	-2.297865	-1.922343
C	-1.513419	-3.139565	-0.988540
H	-1.169342	-3.573639	1.092791
H	-2.001516	-2.528448	-2.979121
O	-3.505660	-0.371453	-2.321939
O	-2.537645	-1.500780	2.129684
O	-0.782256	-4.186916	-1.464688
C	-1.939090	-2.314057	3.103272
H	-2.255346	-1.919161	4.076422
H	-2.267369	-3.363393	3.019075
H	-0.838369	-2.273993	3.044574
C	-3.408999	-0.592670	-3.703984
H	-3.866671	-1.553681	-3.990967
H	-3.953363	0.223630	-4.189560
H	-2.359964	-0.579564	-4.042768
C	-1.240837	-5.473620	-1.115394
H	-2.282254	-5.625981	-1.447489
H	-0.592673	-6.196452	-1.628204
H	-1.181567	-5.657400	-0.030664

C	-5.776498	-0.870613	1.981162
H	-4.945314	-1.588334	2.065073
H	-6.015050	-0.827693	0.906354
C	-7.398495	-2.707718	1.858370
H	-8.212616	-3.269822	2.342697
H	-7.754617	-2.386813	0.866248
H	-6.553323	-3.397558	1.703751
C	-6.589156	-2.034647	4.098481
H	-5.716907	-2.704594	4.029597
H	-6.341096	-1.230596	4.803584
H	-7.421251	-2.610420	4.534648
C	-8.182920	-0.568885	2.844997
H	-7.991772	0.256413	3.546990
H	-8.462016	-0.132133	1.873378
H	-9.053997	-1.125479	3.226576
H	-4.247934	0.795466	-0.495317
N	-6.936449	-0.862553	-3.132738
C	-7.133417	0.366158	-2.512965
N	-7.255640	1.441545	-3.368505
N	-7.199306	0.551366	-1.237799
H	-7.296479	-0.340927	-0.756298
C	-6.467864	-1.955803	-2.321024
H	-6.035759	-2.730481	-2.972611
H	-5.681587	-1.610622	-1.636734
H	-7.273508	-2.435491	-1.728365
C	-7.772152	-1.258078	-4.246773
H	-8.258292	-0.380802	-4.688549
H	-7.181497	-1.764319	-5.028338
H	-8.567138	-1.953779	-3.917568
C	-6.477258	1.546836	-4.580050
H	-7.094735	1.912684	-5.417110
H	-5.635527	2.252354	-4.449454
H	-6.062944	0.571794	-4.855574
C	-7.674205	2.703144	-2.812941
H	-8.117582	3.320480	-3.609500
H	-8.417119	2.534689	-2.024636
H	-6.832498	3.266569	-2.366688

Vibrational frequencies

9.1371	12.6379	14.6409
17.1953	19.0965	20.5593
25.1608	27.2138	28.5597
29.5826	29.9291	32.2621

33.7444 35.4923 37.2617
39.7222 40.1698 42.2772
45.4764 47.0910 48.1585
49.0266 50.8241 55.6029
56.4775 59.3846 64.3986
67.5997 70.5707 71.5992

TSpcet

Zero-point correction= 1.342373
Thermal correction to Energy= 1.438164
Thermal correction to Enthalpy= 1.439108
Thermal correction to Gibbs Free Energy= 1.203587
Sum of electronic and zero-point Energies= -5219.812933
Sum of electronic and thermal Energies= -5219.717141
Sum of electronic and thermal Enthalpies= -5219.716197
Sum of electronic and thermal Free Energies= -5219.951718

Cartesian coordinates

Ir	2.675701	-0.671535	-0.241697
C	4.361078	3.585166	-1.751024
C	3.189153	3.086234	-2.317943
C	2.690228	1.878598	-1.860129
C	4.528971	1.564472	-0.444200
C	5.029291	2.822249	-0.810400
H	4.758760	4.555504	-2.054065
H	1.749613	1.480349	-2.238058
H	5.957434	3.178153	-0.372674
C	5.152006	-1.692586	1.257214
C	4.524252	-0.667991	0.537313
C	5.196089	0.581072	0.399906
C	6.443235	0.751753	1.018857
C	7.057970	-0.253327	1.746819
C	6.389913	-1.469392	1.842825
H	4.694790	-2.674498	1.389764
H	8.026910	-0.091102	2.218043
N	3.334623	1.142076	-0.949033
F	7.094553	1.915235	0.926281
F	6.968342	-2.453150	2.532669
C	2.523734	3.819467	-3.443443
F	1.382476	3.242096	-3.818818
F	3.327351	3.832500	-4.523568
F	2.268607	5.091843	-3.150102
C	-1.511907	1.240952	-1.892449

C	-0.844347	0.267103	-2.692322
C	0.220727	-0.436361	-2.167220
C	-0.016086	0.582324	-0.081758
C	-1.106369	1.332721	-0.577277
H	-1.116390	0.103778	-3.735739
H	0.782011	-1.142176	-2.785831
C	0.493454	1.756312	3.465274
C	-0.128670	1.489905	2.263010
C	0.534844	0.791136	1.227794
C	2.410183	0.563676	2.605581
C	1.810829	1.254634	3.635791
H	-1.144494	1.827829	2.076960
H	3.425497	0.172477	2.708194
H	2.371012	1.416478	4.557066
N	0.677697	-0.267074	-0.915585
N	1.808824	0.332809	1.429157
C	3.472433	-4.021483	-2.697597
C	3.916265	-3.554357	-3.922159
C	4.040229	-2.174910	-4.070366
C	3.731856	-1.279171	-3.057032
C	3.270390	-1.753385	-1.822437
C	3.150012	-3.162784	-1.636836
H	4.156066	-4.241888	-4.732720
H	3.853857	-0.212327	-3.253486
C	2.299407	-5.117604	1.500793
C	2.699673	-4.886062	0.197043
C	2.696237	-3.581182	-0.320593
C	1.894066	-2.769098	1.724176
C	1.869288	-4.038482	2.277841
H	2.324782	-6.126356	1.916422
H	3.039082	-5.707926	-0.427896
H	1.611840	-1.889170	2.301634
F	4.471297	-1.707933	-5.242254
F	3.345829	-5.345309	-2.556251
N	2.308224	-2.543704	0.475410
C	1.366047	-4.224188	3.677004
F	1.931514	-5.272725	4.272452
F	0.033419	-4.439306	3.697760
F	1.584372	-3.148173	4.434534
C	-0.144846	2.590439	4.568808
C	-1.573096	2.997132	4.216462
H	-2.217406	2.113876	4.092940
H	-1.999606	3.610898	5.024205

H	-1.606949	3.583023	3.286413
C	-0.166470	1.788918	5.877423
H	-0.616808	2.389059	6.683728
H	-0.760300	0.868176	5.765699
H	0.844833	1.501238	6.200619
C	0.697065	3.863515	4.752777
H	1.730629	3.626448	5.046502
H	0.733911	4.447349	3.821533
H	0.259133	4.494600	5.542745
H	-1.540461	2.082030	0.079021
C	-2.501735	2.220376	-2.517925
C	-1.723573	3.140515	-3.472010
H	-1.185153	2.567530	-4.241318
H	-2.418763	3.827491	-3.981924
H	-0.990772	3.735546	-2.910511
C	-3.580989	1.470927	-3.306210
H	-4.127646	0.765322	-2.666191
H	-4.299712	2.187877	-3.732925
H	-3.151947	0.898493	-4.142594
C	-3.173119	3.100669	-1.462938
H	-3.704129	2.494978	-0.716613
H	-2.441642	3.730197	-0.935882
H	-3.903528	3.766946	-1.947293
P	0.715689	4.886358	0.276085
F	0.591378	3.919526	-1.033430
F	-0.203748	6.004408	-0.470654
F	-0.641480	4.209564	0.898362
F	0.823253	5.846171	1.590694
F	1.633169	3.766582	1.017456
F	2.055835	5.571164	-0.341760
C	-5.383795	1.275782	1.568498
C	-4.744317	2.455718	2.296116
H	-4.029953	2.110975	3.053185
H	-4.204364	3.089907	1.578340
H	-5.510132	3.070095	2.786228
C	-6.397931	1.783699	0.534190
H	-5.896563	2.415488	-0.212713
H	-6.875896	0.940452	0.020124
H	-7.165587	2.388834	1.031242
C	-6.906265	0.496822	3.692421
N	-4.322558	0.602577	0.854267
C	-4.182640	-0.305125	-0.005188
C	-3.124815	-1.272147	-0.084418

C	-2.359120	-1.619789	1.067392
C	-2.881051	-1.980221	-1.292137
C	-1.460192	-2.682978	1.023752
C	-1.961574	-3.022506	-1.336905
C	-1.278384	-3.376896	-0.174456
H	-0.902266	-2.986955	1.905038
H	-1.762329	-3.585492	-2.245828
O	-3.595387	-1.595218	-2.356964
O	-2.602697	-0.915961	2.178144
O	-0.416211	-4.422844	-0.250859
C	-1.928446	-1.250567	3.369310
H	-2.310994	-0.571166	4.140094
H	-2.132478	-2.291800	3.667353
H	-0.842168	-1.100143	3.268337
C	-3.310320	-2.172965	-3.608423
H	-3.598566	-3.236209	-3.638127
H	-3.895134	-1.617541	-4.348457
H	-2.240805	-2.076654	-3.850573
C	-0.790699	-5.574940	0.476819
H	-1.781934	-5.936609	0.154332
H	-0.040796	-6.346552	0.263013
H	-0.810434	-5.390041	1.562467
C	-5.973248	0.183858	2.501396
H	-5.111974	-0.371632	2.905944
H	-6.497463	-0.519513	1.831743
C	-7.477692	-0.859138	4.130592
H	-8.118204	-0.742747	5.018864
H	-8.085051	-1.312704	3.331269
H	-6.671910	-1.565938	4.385774
C	-6.138731	1.084036	4.882768
H	-5.276499	0.450731	5.146921
H	-5.765169	2.097826	4.689451
H	-6.795878	1.139874	5.765031
C	-8.075678	1.414867	3.331535
H	-7.746594	2.440376	3.107290
H	-8.633864	1.034821	2.461726
H	-8.777399	1.478123	4.178119
H	-5.155598	-0.511616	-0.730213
N	-6.764414	-2.783503	-2.863796
C	-6.703192	-1.485221	-2.436273
N	-6.905481	-0.513655	-3.366857
N	-6.470894	-1.150184	-1.188885
H	-6.557417	-1.947108	-0.561315

C	-6.165453	-3.829869	-2.069110
H	-5.850867	-4.649692	-2.731915
H	-5.276997	-3.451723	-1.548481
H	-6.866744	-4.250137	-1.324419
C	-7.756505	-3.227377	-3.822349
H	-8.376202	-2.384717	-4.148526
H	-7.293766	-3.693277	-4.707740
H	-8.419769	-3.972005	-3.351006
C	-6.527311	-0.654752	-4.754188
H	-7.395251	-0.554932	-5.427018
H	-5.799577	0.129984	-5.020840
H	-6.060092	-1.629526	-4.927933
C	-7.299633	0.816190	-2.965666
H	-8.048265	1.200962	-3.675918
H	-7.738018	0.782324	-1.963142
H	-6.447461	1.516365	-2.954443

Vibrational frequencies

-307.5258	6.5380	14.3252
16.0731	19.0770	20.5664
23.5531	25.4756	28.1228
30.0904	30.7387	32.9767
36.2051	37.5054	38.4417
39.2381	40.1803	41.5042
44.3830	45.7566	48.6082
48.8615	53.2557	55.9976
59.9662	64.6774	65.2232
66.8655	71.5992	73.2931

^{3}M2

Zero-point correction= 1.347626
Thermal correction to Energy= 1.444264
Thermal correction to Enthalpy= 1.445208
Thermal correction to Gibbs Free Energy= 1.207695
Sum of electronic and zero-point Energies= -5219.835460
Sum of electronic and thermal Energies= -5219.738821
Sum of electronic and thermal Enthalpies= -5219.737877
Sum of electronic and thermal Free Energies= -5219.975390

Cartesian coordinates

Ir	3.298709	-0.552633	-0.084442
C	4.399620	3.659008	-2.130870
C	3.267214	2.967792	-2.565419

C	2.957110	1.758601	-1.966946
C	4.852404	1.857233	-0.588776
C	5.190382	3.102993	-1.140533
H	4.663929	4.624290	-2.567280
H	2.072093	1.195404	-2.258243
H	6.080072	3.619698	-0.791834
C	5.774434	-0.958506	1.675868
C	5.074554	-0.162290	0.761113
C	5.612983	1.108330	0.404055
C	6.813552	1.525787	0.997189
C	7.502807	0.746002	1.910706
C	6.959859	-0.495308	2.228703
H	5.409706	-1.942054	1.978898
H	8.432967	1.096538	2.357030
N	3.722807	1.222237	-1.011687
F	7.342682	2.715800	0.695024
F	7.612463	-1.261119	3.103846
C	2.441135	3.488881	-3.703042
F	1.290543	2.831514	-3.834276
F	3.103243	3.354289	-4.866315
F	2.171603	4.786197	-3.568858
C	-1.090959	0.022784	-2.203420
C	-0.192946	-0.957713	-2.726978
C	0.985115	-1.215191	-2.062395
C	0.461392	0.285795	-0.334974
C	-0.754935	0.598971	-0.999169
H	-0.396120	-1.484001	-3.659244
H	1.714400	-1.919793	-2.471982
C	0.536539	2.287151	2.858990
C	0.084151	1.769062	1.666155
C	0.886461	0.895655	0.882189
C	2.606079	1.095373	2.469826
C	1.852796	1.921126	3.273388
H	-0.905384	2.024605	1.296524
H	3.625684	0.815770	2.749554
H	2.285629	2.292461	4.202628
N	1.339345	-0.609707	-0.916938
N	2.160493	0.586078	1.310821
C	4.751744	-4.053595	-1.969476
C	5.301677	-3.681142	-3.182688
C	5.288275	-2.324048	-3.499304
C	4.750513	-1.360958	-2.658601
C	4.188894	-1.740392	-1.432956

C	4.199092	-3.121960	-1.077302
H	5.723910	-4.423150	-3.859732
H	4.773371	-0.317542	-2.979143
C	2.863985	-4.841913	2.030901
C	3.514201	-4.698493	0.818297
C	3.592379	-3.436760	0.205099
C	2.428767	-2.487213	2.008110
C	2.294144	-3.715381	2.633165
H	2.796870	-5.822303	2.506513
H	3.961292	-5.559173	0.328358
H	2.034788	-1.569780	2.445989
F	5.815955	-1.949886	-4.664102
F	4.754200	-5.357206	-1.670009
N	3.056942	-2.351567	0.836452
C	1.499958	-3.838869	3.897695
F	2.114319	-4.609658	4.795862
F	0.301825	-4.399240	3.659998
F	1.270091	-2.651439	4.462945
C	-0.292959	3.220985	3.733303
C	-1.677031	3.478340	3.141375
H	-2.248326	2.544389	3.035517
H	-2.247852	4.145103	3.806230
H	-1.609841	3.949496	2.152514
C	-0.456418	2.591980	5.124642
H	-1.047224	3.256084	5.775631
H	-0.980917	1.625396	5.060548
H	0.512550	2.417566	5.615845
C	0.440281	4.565609	3.854947
H	1.442913	4.446862	4.292717
H	0.544693	5.029557	2.863856
H	-0.130254	5.251337	4.502010
H	-1.383972	1.374191	-0.569906
C	-2.289958	0.486445	-3.024739
C	-1.753355	1.375995	-4.159279
H	-1.019361	0.836100	-4.777407
H	-2.580604	1.697473	-4.813655
H	-1.268988	2.272917	-3.748380
C	-3.032524	-0.709970	-3.631272
H	-3.404561	-1.384570	-2.847890
H	-3.892298	-0.356193	-4.222080
H	-2.394230	-1.298379	-4.306542
C	-3.268855	1.308014	-2.184369
H	-3.633701	0.740087	-1.315456

H	-2.809955	2.234880	-1.816367
H	-4.134765	1.593511	-2.801465
P	-0.706788	4.742102	-0.919682
F	0.432535	3.585682	-1.045059
F	-1.274792	4.348233	-2.396896
F	-1.741096	3.656216	-0.246736
F	-1.854428	5.887724	-0.787429
F	-0.155719	5.123860	0.567110
F	0.305740	5.824302	-1.581312
C	-5.500542	1.044887	1.872700
C	-5.264482	2.390708	1.177719
H	-4.202470	2.672241	1.216284
H	-5.549309	2.311302	0.117657
H	-5.859585	3.192392	1.629442
C	-6.977098	0.668036	1.805987
H	-7.304519	0.589334	0.760678
H	-7.164180	-0.296674	2.300271
H	-7.594652	1.437046	2.288938
C	-5.513092	1.742436	4.521493
N	-4.668316	0.093281	1.161127
C	-4.803856	-1.000242	0.603639
C	-3.757432	-1.907964	0.175059
C	-2.488917	-1.932298	0.812301
C	-3.991352	-2.849771	-0.854173
C	-1.494175	-2.829140	0.408470
C	-3.003355	-3.729400	-1.276318
C	-1.750141	-3.701898	-0.650092
H	-0.523614	-2.815723	0.894649
H	-3.153439	-4.431003	-2.093791
O	-5.217777	-2.815501	-1.416733
O	-2.306528	-1.078645	1.823096
O	-0.843632	-4.563546	-1.135063
C	-1.195615	-1.238461	2.672274
H	-1.303197	-0.489289	3.465315
H	-1.175536	-2.247382	3.114269
H	-0.252588	-1.042857	2.140362
C	-5.557542	-3.801196	-2.362478
H	-5.400383	-4.815073	-1.961334
H	-6.623166	-3.671936	-2.585460
H	-4.978178	-3.684359	-3.292783
C	0.436776	-4.598223	-0.554239
H	0.390122	-4.902963	0.504115
H	1.019391	-5.338957	-1.114751

H	0.935129	-3.618741	-0.628583
C	-4.918405	0.987077	3.310481
H	-3.863049	1.282804	3.206137
H	-4.890535	-0.081038	3.584544
C	-4.455953	1.630778	5.629556
H	-4.816399	2.093638	6.561825
H	-4.218201	0.576644	5.845603
H	-3.521116	2.134011	5.339798
C	-5.772691	3.226779	4.257269
H	-4.883674	3.726485	3.843049
H	-6.610003	3.383324	3.561176
H	-6.035130	3.734555	5.199193
C	-6.797618	1.086214	5.040586
H	-7.641101	1.196627	4.346335
H	-6.645952	0.010067	5.221528
H	-7.097790	1.547327	5.995135
N	-9.530424	-2.141221	-1.899812
C	-8.322094	-1.601288	-1.653230
N	-7.668405	-0.938391	-2.619622
N	-7.774727	-1.732392	-0.448327
H	-8.352924	-1.954216	0.351276
C	-10.035614	-3.234129	-1.092953
H	-10.660638	-3.879811	-1.725324
H	-9.203862	-3.835694	-0.705986
H	-10.652625	-2.877620	-0.250269
C	-10.493074	-1.498950	-2.776765
H	-10.127545	-0.513958	-3.086570
H	-10.702826	-2.106064	-3.670691
H	-11.434653	-1.354669	-2.225024
C	-7.785665	-1.300404	-4.020490
H	-8.279724	-0.510803	-4.607010
H	-6.775722	-1.454229	-4.430217
H	-8.346051	-2.235363	-4.130024
C	-6.619134	0.011938	-2.304470
H	-6.628656	0.809311	-3.059979
H	-6.794788	0.465937	-1.322917
H	-5.630114	-0.467612	-2.300787
H	-6.763939	-1.628905	-0.284389

Vibrational frequencies

10.0484	12.4824	16.2961
18.2578	19.0548	21.0682
24.7642	26.5902	27.9425

29.9617 31.5823 32.7370
36.4706 37.3471 38.5705
42.2114 44.5800 46.7188
47.7633 49.6464 51.6392
52.6771 58.0705 59.1118
62.2832 65.9676 66.9632
71.6748 74.6753 76.4882

M3

Zero-point correction= 0.433579
Thermal correction to Energy= 0.458480
Thermal correction to Enthalpy= 0.459425
Thermal correction to Gibbs Free Energy= 0.378226
Sum of electronic and zero-point Energies= -980.873996
Sum of electronic and thermal Energies= -980.849095
Sum of electronic and thermal Enthalpies= -980.848151
Sum of electronic and thermal Free Energies= -980.929350

Cartesian coordinates

C	-2.076001	-1.133032	-0.124014
C	-2.899702	-2.410850	-0.235248
H	-3.491318	-2.417565	-1.161847
H	-2.227485	-3.282359	-0.252132
H	-3.578255	-2.525923	0.621025
C	-1.266626	-1.135686	1.170534
H	-0.520941	-1.945231	1.142927
H	-0.730296	-0.186683	1.312443
H	-1.911098	-1.298523	2.043342
N	-1.159163	-1.149383	-1.308888
C	0.010283	-0.789139	-1.320440
C	1.157969	-0.241181	-0.709771
C	2.233986	-1.067668	-0.303319
C	1.319333	1.167779	-0.600999
C	3.421517	-0.523230	0.187641
C	2.499303	1.714738	-0.115689
C	3.550633	0.869105	0.272602
H	4.230644	-1.176306	0.504332
H	2.640666	2.789638	-0.015176
O	0.249052	1.889553	-0.983552
O	1.999463	-2.389500	-0.410677
O	4.658104	1.488679	0.728683
C	3.008326	-3.295918	-0.041683
H	2.607946	-4.300238	-0.225036

H	3.920108	-3.156893	-0.646354
H	3.266638	-3.202140	1.026465
C	0.306613	3.291138	-0.895349
H	1.107618	3.704035	-1.530933
H	-0.661806	3.665724	-1.248605
H	0.464961	3.624756	0.143891
C	5.752139	0.710915	1.141618
H	6.149496	0.094564	0.317158
H	6.530286	1.411668	1.468153
H	5.488589	0.051113	1.985866
C	-2.879060	0.167776	-0.344826
H	-3.156333	0.179550	-1.412815
H	-2.148183	0.985021	-0.224018
C	-3.972694	0.435850	1.967302
H	-3.884896	-0.608859	2.299773
H	-3.078805	0.980395	2.309270
H	-4.846587	0.868226	2.480685
C	-4.434022	2.010601	0.103814
H	-4.557349	2.143553	-0.982969
H	-5.357108	2.358633	0.594054
H	-3.608582	2.663011	0.430868
C	-4.149832	0.542712	0.451716
C	-5.367703	-0.283283	0.023611
H	-5.509232	-0.243085	-1.068108
H	-5.283699	-1.338825	0.313980
H	-6.280553	0.114800	0.495353

Vibrational frequencies

16.1095	25.3413	29.1953
45.3040	65.2035	84.3856
91.3944	113.2390	120.7853
133.8129	174.5269	188.5385
192.3265	210.0042	215.4240
241.0503	246.6775	251.8151
265.6885	275.8339	280.6973
291.2846	294.2291	302.0053
309.9580	313.1399	331.6524
343.0544	355.3141	368.4515

TMG$^{\bullet}$H^{+}+Ir^{II-}

Zero-point correction= 0.910686

Thermal correction to Energy= 0.981552

Thermal correction to Enthalpy= 0.982496

Thermal correction to Gibbs Free Energy= 0.794067
Sum of electronic and zero-point Energies= -4238.913124
Sum of electronic and thermal Energies= -4238.842259
Sum of electronic and thermal Enthalpies= -4238.841315
Sum of electronic and thermal Free Energies= -4239.029743

Cartesian coordinates

Ir	2.140966	-0.771433	-0.294805
C	3.254954	3.753992	-1.478004
C	2.013647	3.237233	-1.846417
C	1.704589	1.935030	-1.493480
C	3.798739	1.619491	-0.492390
C	4.147271	2.943842	-0.797852
H	3.529341	4.783319	-1.720916
H	0.735031	1.497093	-1.737467
H	5.125023	3.325134	-0.509357
C	4.819159	-1.693570	0.880768
C	4.052336	-0.672519	0.304594
C	4.638764	0.618398	0.159777
C	5.947006	0.827504	0.611277
C	6.700243	-0.174728	1.196474
C	6.108946	-1.429016	1.312421
H	4.418663	-2.702647	1.008555
H	7.716794	0.011077	1.541262
N	2.564787	1.153721	-0.843231
F	6.520200	2.028972	0.499974
F	6.821573	-2.414669	1.863029
C	1.052246	4.056931	-2.670600
F	-0.153603	3.501324	-2.741282
F	1.504182	4.185276	-3.924483
F	0.920851	5.291837	-2.179331
C	-2.507233	0.357120	-1.418401
C	-1.741444	-0.441216	-2.328468
C	-0.482009	-0.850850	-1.966674
C	-0.639409	0.156980	0.149133
C	-1.942392	0.620840	-0.191074
H	-2.122724	-0.708499	-3.317123
H	0.141468	-1.423698	-2.658155
C	0.073293	1.329760	3.662303
C	-0.603390	1.102953	2.484089
C	0.009740	0.436610	1.386101
C	1.986038	0.251313	2.645453
C	1.417840	0.872160	3.738498

H	-1.623340	1.460160	2.354438
H	3.018506	-0.094782	2.665921
H	2.023972	1.016385	4.633087
N	0.086494	-0.557738	-0.786186
N	1.323151	0.024258	1.500319
C	2.959072	-3.753655	-3.186342
C	3.416428	-3.115724	-4.330422
C	3.515030	-1.726976	-4.294290
C	3.179163	-0.983053	-3.168198
C	2.722729	-1.625109	-2.015789
C	2.612248	-3.047365	-2.023014
H	3.674626	-3.688152	-5.221600
H	3.290367	0.102272	-3.220659
C	1.502965	-5.424061	0.724670
C	1.965896	-5.010462	-0.514668
C	2.138272	-3.643200	-0.783267
C	1.407472	-3.123882	1.386563
C	1.212715	-4.458997	1.696163
H	1.374970	-6.486952	0.936100
H	2.193835	-5.742146	-1.285523
H	1.200706	-2.328365	2.105158
F	3.947527	-1.105272	-5.388803
F	2.863473	-5.087041	-3.226126
N	1.855788	-2.728400	0.188372
C	0.696175	-4.868148	3.041441
F	1.498459	-5.770608	3.620097
F	-0.515562	-5.431647	2.949530
F	0.588895	-3.829601	3.871667
C	-0.545127	2.074518	4.835701
C	-2.012418	2.423862	4.593794
H	-2.624595	1.517156	4.447766
H	-2.413889	2.956475	5.472672
H	-2.141280	3.070180	3.714457
C	-0.438973	1.206357	6.099489
H	-0.871737	1.740887	6.963628
H	-0.993706	0.265055	5.970096
H	0.599363	0.958585	6.351004
C	0.238943	3.381569	5.043133
H	1.300297	3.188222	5.245947
H	0.156318	4.010851	4.141806
H	-0.170952	3.943571	5.898923
H	-2.454711	1.265563	0.517860
C	-3.835162	0.958694	-1.853378

C	-3.533048	2.048476	-2.884796
H	-2.989714	1.647367	-3.756680
H	-4.469448	2.506402	-3.252938
H	-2.919120	2.843683	-2.432530
C	-4.722375	-0.123310	-2.485539
H	-4.933873	-0.936725	-1.773340
H	-5.685339	0.319147	-2.801041
H	-4.266690	-0.573646	-3.384326
C	-4.591485	1.582170	-0.683448
H	-4.785701	0.845074	0.108957
H	-4.032215	2.420504	-0.240200
H	-5.560609	1.967325	-1.028720
P	-1.641961	4.647082	0.702166
F	-0.585797	3.535335	0.164939
F	-2.484525	4.529769	-0.684612
F	-2.569872	3.456979	1.349067
F	-2.713288	5.745592	1.257312
F	-0.817271	4.755743	2.107118
F	-0.736371	5.837908	0.079452
N	-10.155558	-2.939797	-0.659097
C	-9.022397	-2.457628	-0.126495
N	-8.590118	-1.224217	-0.427728
N	-8.316636	-3.210491	0.721580
H	-8.732496	-3.990202	1.209982
C	-10.395499	-4.372283	-0.737593
H	-10.966264	-4.581843	-1.655035
H	-9.448780	-4.916252	-0.783598
H	-10.983701	-4.736774	0.124145
C	-11.289369	-2.089463	-0.957535
H	-11.120100	-1.074561	-0.582079
H	-11.496055	-2.046068	-2.038404
H	-12.180607	-2.495759	-0.453022
C	-8.798909	-0.635203	-1.743967
H	-9.453879	0.248658	-1.691248
H	-7.816780	-0.324214	-2.144200
H	-9.225661	-1.365991	-2.429925
C	-7.657167	-0.525459	0.442778
H	-7.828886	0.552674	0.334561
H	-7.839568	-0.801439	1.494444
H	-6.607400	-0.735762	0.178308
H	-7.344269	-3.004219	0.915202

Vibrational frequencies

3.5987 10.7763 14.8427
16.4524 18.7208 20.3691
21.8271 25.1969 26.6793
26.9808 29.3156 33.3937
34.7693 35.2852 37.8476
42.9042 44.7660 50.1367
54.8270 57.6248 66.7004
68.9784 70.1463 72.6262
74.8369 78.8918 81.6061
86.3938 87.7095 95.3849

TS2

Zero-point correction= 0.430024
Thermal correction to Energy= 0.455514
Thermal correction to Enthalpy= 0.456458
Thermal correction to Gibbs Free Energy= 0.372354
Sum of electronic and zero-point Energies= -980.861503
Sum of electronic and thermal Energies= -980.836014
Sum of electronic and thermal Enthalpies= -980.835069
Sum of electronic and thermal Free Energies= -980.919173

Cartesian coordinates

C	2.378837	1.221296	-0.076223
C	3.152833	2.434811	-0.491608
H	3.721748	2.253644	-1.415155
H	2.471457	3.282408	-0.666813
H	3.865334	2.747742	0.291687
C	1.478498	1.420139	1.105261
H	0.788133	2.261766	0.932479
H	0.877044	0.522124	1.311691
H	2.053097	1.652166	2.017902
N	1.124118	1.128965	-1.571345
C	0.029490	0.737028	-1.317039
C	-1.168759	0.233190	-0.792211
C	-2.231551	1.099356	-0.436057
C	-1.354136	-1.168171	-0.634017
C	-3.437552	0.594307	0.051314
C	-2.552848	-1.672786	-0.150046
C	-3.593081	-0.791579	0.186715
H	-4.242051	1.272629	0.323359
H	-2.719135	-2.740170	-0.015151
O	-0.292598	-1.920116	-0.969514
O	-1.971038	2.408545	-0.590012

O	-4.719090	-1.371120	0.643921
C	-2.963771	3.348813	-0.260584
H	-2.537581	4.337259	-0.469254
H	-3.870476	3.211303	-0.872792
H	-3.236098	3.292330	0.806482
C	-0.373418	-3.316851	-0.825728
H	-1.168650	-3.742429	-1.459870
H	0.595638	-3.718715	-1.145099
H	-0.555842	-3.604814	0.222974
C	-5.805665	-0.558451	1.009616
H	-6.177403	0.033309	0.155993
H	-6.601402	-1.232948	1.348348
H	-5.542565	0.126736	1.833266
C	2.997465	-0.140489	-0.271869
H	3.286839	-0.222743	-1.334657
H	2.195969	-0.884404	-0.119216
C	3.949299	-0.500962	2.070021
H	3.870876	0.543853	2.404892
H	3.015240	-1.016700	2.344216
H	4.770757	-0.967188	2.637656
C	4.464668	-2.066622	0.206017
H	4.654177	-2.182387	-0.873190
H	5.337653	-2.464498	0.747718
H	3.592917	-2.690009	0.462546
C	4.218186	-0.597511	0.567619
C	5.475742	0.203303	0.222070
H	5.676775	0.179640	-0.860892
H	5.392111	1.255633	0.526958
H	6.353606	-0.220068	0.736427

Vibrational frequencies

-501.3947	8.5060	15.6234
23.5534	34.0774	60.5036
82.9517	85.6023	110.2217
119.3498	127.7163	173.8591
178.0428	191.0223	198.1913
200.3404	211.4279	221.5196
224.5361	244.5173	259.8413
264.1637	273.8473	275.6732
288.4834	291.5929	300.0680
314.7284	322.0365	330.0699

aromatic nitrile

Zero-point correction= 0.198599
Thermal correction to Energy= 0.212336
Thermal correction to Enthalpy= 0.213280
Thermal correction to Gibbs Free Energy= 0.158493
Sum of electronic and zero-point Energies= -666.654348
Sum of electronic and thermal Energies= -666.640611
Sum of electronic and thermal Enthalpies= -666.639667
Sum of electronic and thermal Free Energies= -666.694455

Cartesian coordinates

C	-0.045628	-1.621261	-0.000029
C	1.242084	-1.063642	-0.000061
C	1.438540	0.322787	-0.000057
C	0.322879	1.163389	-0.000016
C	-0.981368	0.624023	0.000018
C	-1.153133	-0.782369	0.000010
H	-0.136582	-2.705511	-0.000039
H	2.440389	0.742622	-0.000089
O	-2.419186	-1.208500	0.000039
O	0.398911	2.496724	-0.000012
O	2.247978	-1.945951	-0.000095
C	3.578361	-1.482328	-0.000167
H	3.796953	-0.882767	0.898611
H	4.217197	-2.373237	-0.000215
H	3.796848	-0.882745	-0.898955
C	1.663123	3.119941	0.000073
H	1.474313	4.199585	0.000168
H	2.242103	2.854141	0.899293
H	2.242141	2.854309	-0.899174
C	-2.678003	-2.593987	0.000105
H	-2.264237	-3.079123	0.898883
H	-3.768512	-2.704458	0.000179
H	-2.264353	-3.079187	-0.898691
C	-2.111075	1.482769	0.000065
N	-3.036081	2.186038	0.000131

Vibrational frequencies

62.4860	81.6599	110.7945
123.8637	134.7839	177.8034
190.5705	192.5831	207.7178
244.3907	266.0899	284.2926
295.1653	309.1805	372.2828

401.7704 453.6232 489.0776
552.8936 559.4277 611.3003
635.5397 669.7695 723.2386
751.1545 762.0696 817.8589
833.4206 984.1790 1007.3652

M4

Zero-point correction= 0.229587
Thermal correction to Energy= 0.240913
Thermal correction to Enthalpy= 0.241857
Thermal correction to Gibbs Free Energy= 0.192990
Sum of electronic and zero-point Energies= -314.224565
Sum of electronic and thermal Energies= -314.213239
Sum of electronic and thermal Enthalpies= -314.212294
Sum of electronic and thermal Free Energies= -314.261161

Cartesian coordinates

C	-1.462012	-0.000057	-0.318256
C	-2.146336	-1.274056	0.043005
H	-2.218448	-1.415158	1.140400
H	-3.189136	-1.291009	-0.326694
H	-1.627607	-2.154599	-0.364079
C	-2.145466	1.274420	0.042935
H	-1.628795	2.154280	-0.368294
H	-3.189806	1.289944	-0.322302
H	-2.212875	1.418197	1.140317
C	1.123098	-0.000096	0.013788
C	-0.105347	-0.000560	-0.941247
H	-0.004931	-0.887010	-1.594521
H	-0.004714	0.885112	-1.595544
C	1.112184	1.248602	0.896012
H	0.229853	1.268496	1.553464
H	2.007776	1.278918	1.537392
H	1.102533	2.167572	0.287939
C	2.387903	-0.001371	-0.846334
H	3.292924	-0.000989	-0.217851
H	2.426888	-0.892366	-1.493541
H	2.427427	0.888260	-1.495384
C	1.111312	-1.247012	0.898504
H	1.101292	-2.167208	0.292291
H	2.006763	-1.276538	1.540120
H	0.228837	-1.265126	1.555837

Vibrational frequencies

46.5769	91.2524	108.0671
139.6203	179.8181	234.1683
273.7211	276.4738	298.1946
302.2859	311.7879	377.4272
391.9406	416.1766	441.8999
511.9078	740.8700	809.6392
896.0215	913.8664	932.9771
944.1751	944.6731	948.5219
963.2633	1004.5806	1017.9204
1037.1352	1038.0047	1147.0229

R2

Zero-point correction= 0.367040
Thermal correction to Energy= 0.391172
Thermal correction to Enthalpy= 0.392116
Thermal correction to Gibbs Free Energy= 0.312708
Sum of electronic and zero-point Energies= -1051.215254
Sum of electronic and thermal Energies= -1051.191122
Sum of electronic and thermal Enthalpies= -1051.190178
Sum of electronic and thermal Free Energies= -1051.269586

Cartesian coordinates

C	-0.654165	-1.407785	-0.730861
N	0.265989	-0.384488	-0.373745
C	-0.559357	-2.089857	-1.873487
H	0.220983	-1.861161	-2.601778
H	-1.251724	-2.905297	-2.082050
C	-1.680515	-1.700641	0.312575
O	-1.627515	-1.264025	1.437521
O	-2.653051	-2.484347	-0.135479
C	-3.664125	-2.830383	0.800886
H	-4.195011	-1.930585	1.143995
H	-4.354305	-3.497412	0.273454
H	-3.230302	-3.341969	1.671570
C	1.609990	-0.754667	-0.171839
C	-0.251710	0.875281	-0.014913
O	1.936800	-1.904856	-0.015540
O	0.318242	1.696352	0.652152
O	2.400462	0.293336	-0.233970
O	-1.468387	0.979625	-0.531985
C	3.812852	0.220383	0.133824
C	3.941738	-0.278058	1.565926

H	3.626496	-1.325094	1.656872
H	4.990633	-0.200019	1.886035
H	3.328202	0.339958	2.238137
C	4.556561	-0.659580	-0.860243
H	5.634448	-0.623829	-0.644707
H	4.217357	-1.700857	-0.797115
H	4.399995	-0.293257	-1.885853
C	-2.381242	2.058751	-0.160927
C	-2.581123	2.076394	1.347920
H	-1.665985	2.385300	1.868064
H	-3.383490	2.785677	1.597237
H	-2.869547	1.077566	1.705295
C	-3.665679	1.664475	-0.872036
H	-4.445436	2.416483	-0.686752
H	-3.499168	1.591795	-1.956576
H	-4.024866	0.690278	-0.508625
C	-1.842350	3.378534	-0.691811
H	-0.897358	3.641438	-0.200222
H	-1.676566	3.316134	-1.777589
H	-2.574219	4.176837	-0.500600
C	4.261140	1.668267	0.023295
H	3.678462	2.302608	0.706254
H	5.325866	1.753473	0.282291
H	4.119107	2.037985	-1.002561

Vibrational frequencies

18.4884	24.9622	41.9683
44.9086	57.5622	80.5227
95.7617	111.5189	117.0321
124.4411	131.9135	148.0094
158.8083	201.0405	213.1624
217.3229	217.5413	239.8892
247.1586	261.5444	263.6664
277.2321	282.4754	310.3550
325.3566	336.2287	352.3664
356.7500	357.2099	397.3743

TS3

Zero-point correction= 0.600078

Thermal correction to Energy= 0.634833

Thermal correction to Enthalpy= 0.635777

Thermal correction to Gibbs Free Energy= 0.533725

Sum of electronic and zero-point Energies= -1365.379307

Sum of electronic and thermal Energies= -1365.344552
Sum of electronic and thermal Enthalpies= -1365.343608
Sum of electronic and thermal Free Energies= -1365.445660

Cartesian coordinates

C	-2.745551	1.106844	-0.838112
H	-1.903819	1.807669	-0.721622
H	-3.281645	1.368080	-1.782512
H	-3.437697	1.261329	-0.004722
C	-1.143473	-0.453596	-1.968026
H	-0.338518	0.282677	-1.820626
H	-0.702800	-1.463939	-1.971697
H	-1.586863	-0.281360	-2.976424
C	-1.233646	-0.613960	0.759348
H	-2.084098	-0.451323	1.438911
H	-1.026403	-1.675794	0.513518
C	-0.114995	0.201382	1.022012
C	-0.166771	1.421688	1.828755
O	0.809733	2.070674	2.169075
O	-1.414390	1.777742	2.160274
C	-1.546725	2.965094	2.922144
H	-1.164633	3.830501	2.365352
H	-2.619825	3.088316	3.114956
H	-0.999878	2.886944	3.875013
N	1.174315	-0.100697	0.512791
C	1.913817	0.900650	-0.150259
C	1.745383	-1.360818	0.773615
O	3.113798	0.940728	-0.216300
O	1.406168	-2.042292	1.712345
O	1.065590	1.770474	-0.682809
O	2.612617	-1.687102	-0.162238
C	1.510745	3.025023	-1.277704
C	3.486362	-2.849867	-0.056528
C	2.650682	-4.122219	-0.107864
H	3.317898	-4.995693	-0.147950
H	2.001190	-4.204071	0.768955
H	2.023119	-4.129066	-1.016580
C	4.320102	-2.751825	1.209725
H	3.698452	-2.846776	2.108871
H	5.070623	-3.561919	1.215809
H	4.849927	-1.788294	1.241318
C	4.361895	-2.724249	-1.292558
H	5.074768	-3.559617	-1.336412

H	3.748984	-2.745955	-2.206894
H	4.923841	-1.779785	-1.268788
C	2.340906	3.820868	-0.277769
H	3.307617	3.338344	-0.089638
H	2.522263	4.828292	-0.680205
H	1.802778	3.905615	0.674600
C	2.271610	2.727592	-2.559597
H	2.533453	3.666288	-3.063001
H	3.192453	2.173004	-2.346347
H	1.643886	2.135143	-3.243117
C	0.201085	3.746203	-1.567546
H	0.399025	4.715820	-2.045572
H	-0.426634	3.144014	-2.246757
H	-0.356658	3.914007	-0.637105
C	-2.233695	-0.305791	-0.929143
C	-3.249615	-1.434828	-1.082225
H	-3.438844	-1.493499	-2.183541
H	-2.721965	-2.383432	-0.849147
C	-4.633709	-1.478072	-0.396311
C	-5.209670	-2.881124	-0.653357
H	-6.206956	-2.980124	-0.199095
H	-5.303630	-3.081507	-1.733638
H	-4.563278	-3.665015	-0.220353
C	-4.528669	-1.279483	1.120754
H	-4.172210	-0.278634	1.386473
H	-5.516256	-1.411767	1.589413
H	-3.842899	-2.016759	1.571456
C	-5.617094	-0.468671	-0.991299
H	-5.332239	0.575791	-0.790208
H	-5.702006	-0.589682	-2.079937
H	-6.622709	-0.619788	-0.563394

Vibrational frequencies

-398.8832	16.8027	23.9008
32.5068	40.9012	44.1574
49.3599	54.5667	60.7522
81.0903	91.9793	98.7372
107.9645	115.2435	131.5955
141.3480	155.3782	161.3719
173.8832	179.6710	191.8781
209.9736	214.2130	219.9243
226.3934	230.0926	244.3072
248.7164	255.9192	275.4736

M5

Zero-point correction= 0.604179
Thermal correction to Energy= 0.639006
Thermal correction to Enthalpy= 0.639950
Thermal correction to Gibbs Free Energy= 0.537670
Sum of electronic and zero-point Energies= -1365.488509
Sum of electronic and thermal Energies= -1365.453683
Sum of electronic and thermal Enthalpies= -1365.452738
Sum of electronic and thermal Free Energies= -1365.555019

Cartesian coordinates

C	-2.131085	0.753547	-1.270703
H	-1.182950	1.311062	-1.284945
H	-2.540069	0.757049	-2.292447
H	-2.824271	1.299294	-0.616600
C	-0.798041	-1.296615	-1.681166
H	0.139470	-0.724841	-1.633916
H	-0.582033	-2.335478	-1.383202
H	-1.125399	-1.310026	-2.732629
C	-1.386041	-0.686414	0.686709
H	-2.215038	-0.423618	1.348378
H	-1.087107	-1.715537	0.936957
C	-0.270185	0.245041	0.992524
C	-0.467822	1.526902	1.658657
O	0.434474	2.250541	2.037851
O	-1.761931	1.828882	1.821331
C	-2.040326	3.060684	2.464185
H	-1.648989	3.903802	1.875807
H	-3.131360	3.128052	2.538140
H	-1.589399	3.090897	3.466465
N	1.048279	-0.056223	0.647431
C	1.919047	0.944964	0.129556
C	1.541398	-1.362501	0.848598
O	3.094346	0.982434	0.372103
O	1.100788	-2.095767	1.698042
O	1.234627	1.749907	-0.660316
O	2.464389	-1.639255	-0.047048
C	1.826052	2.960880	-1.232890
C	3.293784	-2.840990	0.032714
C	2.425009	-4.070927	-0.184756
H	3.064700	-4.963048	-0.250653
H	1.714972	-4.206142	0.640449
H	1.864759	-3.979424	-1.127297

C	4.022771	-2.866414	1.367810
H	3.325259	-3.006441	2.203359
H	4.744116	-3.696069	1.372374
H	4.574695	-1.926582	1.516138
C	4.269217	-2.649509	-1.116440
H	4.963375	-3.499991	-1.165439
H	3.729733	-2.581634	-2.072331
H	4.849984	-1.726541	-0.976480
C	2.380592	3.850423	-0.129869
H	3.262291	3.401632	0.343694
H	2.669465	4.818556	-0.563932
H	1.616228	4.019737	0.640975
C	2.885971	2.557278	-2.246737
H	3.273014	3.455447	-2.749537
H	3.722185	2.041326	-1.758071
H	2.453216	1.894586	-3.010994
C	0.640861	3.624470	-1.914246
H	0.964412	4.551840	-2.407315
H	0.206186	2.958546	-2.673601
H	-0.137277	3.872408	-1.177683
C	-1.884147	-0.677172	-0.792243
C	-3.122029	-1.599237	-0.903000
H	-3.208579	-1.892073	-1.964303
H	-2.858866	-2.530359	-0.369789
C	-4.552861	-1.201176	-0.459834
C	-5.376541	-2.496310	-0.493224
H	-6.429129	-2.298282	-0.235333
H	-5.355350	-2.954567	-1.495201
H	-4.985084	-3.235634	0.223635
C	-4.632294	-0.624402	0.956029
H	-4.206343	-1.316422	1.699611
H	-4.108906	0.339034	1.045431
H	-5.685700	-0.453135	1.230636
C	-5.203283	-0.216815	-1.439728
H	-4.740018	0.777373	-1.407757
H	-5.137205	-0.588154	-2.474980
H	-6.270771	-0.091268	-1.197023

Vibrational frequencies

20.4911	25.8156	26.8122
39.5681	41.0859	48.2296
50.7812	58.3119	63.7669
97.3094	101.0222	108.9390

119.8845 127.2863 147.7295
150.6051 162.9048 176.6113
184.4215 203.8122 209.8787
214.2828 216.2665 226.6691
240.1913 248.7037 253.6610
259.1402 263.1521 274.3798

TS4

Zero-point correction= 0.805273
Thermal correction to Energy= 0.850582
Thermal correction to Enthalpy= 0.851526
Thermal correction to Gibbs Free Energy= 0.727807
Sum of electronic and zero-point Energies= -1727.651406
Sum of electronic and thermal Energies= -1727.606098
Sum of electronic and thermal Enthalpies= -1727.605153
Sum of electronic and thermal Free Energies= -1727.728872

Cartesian coordinates

C	2.785571	-0.586385	1.354897
H	1.820615	-0.611407	1.880522
H	3.452743	-1.293465	1.870927
H	3.208112	0.420393	1.459369
C	1.955000	-2.387852	-0.136512
H	0.994009	-2.403097	0.393730
H	1.788461	-2.726357	-1.171760
H	2.611576	-3.122702	0.354859
C	1.717270	0.001880	-0.891332
H	2.261654	0.938352	-1.047511
H	1.537081	-0.418729	-1.889853
C	0.359508	0.419132	-0.329089
C	0.360443	1.405151	0.816430
O	-0.564126	1.553003	1.579470
O	1.439094	2.173134	0.814382
C	1.555919	3.115715	1.878300
H	1.678058	2.585989	2.833284
H	2.447975	3.710558	1.657839
H	0.665694	3.755618	1.934104
N	-0.642435	-0.596731	-0.154216
C	-1.341295	-0.859148	1.072695
C	-1.004156	-1.331293	-1.286037
O	-2.540338	-0.817249	1.142920
O	-0.690508	-0.996844	-2.403663
O	-0.495835	-1.206186	2.012547

O	-1.669511	-2.411570	-0.932330
C	-0.943483	-1.550201	3.372257
C	-2.208775	-3.360067	-1.909419
C	-1.058720	-4.003005	-2.669727
H	-1.450239	-4.802350	-3.315234
H	-0.536600	-3.269750	-3.297147
H	-0.339749	-4.450350	-1.967440
C	-3.191621	-2.650744	-2.828679
H	-2.687156	-1.903806	-3.454374
H	-3.668133	-3.391520	-3.486693
H	-3.981490	-2.158937	-2.241672
C	-2.919237	-4.373257	-1.028559
H	-3.370766	-5.158648	-1.650477
H	-2.209881	-4.842021	-0.331215
H	-3.713273	-3.885333	-0.445123
C	-1.682280	-0.373968	3.990981
H	-2.636905	-0.186649	3.484541
H	-1.884273	-0.599266	5.048026
H	-1.068827	0.535619	3.935264
C	-1.796356	-2.807180	3.297026
H	-2.047311	-3.136259	4.315592
H	-2.728534	-2.622826	2.748562
H	-1.242384	-3.617096	2.799727
C	0.360860	-1.817621	4.102537
H	0.148481	-2.134417	5.133096
H	0.930333	-2.614049	3.602289
H	0.981652	-0.910998	4.139695
C	2.604156	-0.996452	-0.105194
C	3.945257	-1.133347	-0.873507
H	4.388642	-2.096315	-0.566080
H	3.675081	-1.269711	-1.935845
C	5.101398	-0.102055	-0.816987
C	6.071153	-0.502637	-1.937864
H	6.955937	0.153559	-1.944063
H	6.421447	-1.539183	-1.807846
H	5.588672	-0.431544	-2.925668
C	4.667672	1.345287	-1.063057
H	4.139890	1.450808	-2.024164
H	4.013026	1.728903	-0.266290
H	5.553927	1.998886	-1.101719
C	5.873966	-0.177481	0.506100
H	5.292771	0.195800	1.358904
H	6.173759	-1.213855	0.729105

H	6.791809	0.428900	0.442879
N	-2.780458	2.167204	-0.768540
C	-1.728664	2.900114	-1.188917
N	-1.612681	4.193761	-0.812364
N	-0.851933	2.310963	-2.004966
H	-0.077185	1.093344	-1.183176
C	-3.302690	1.059453	-1.547582
H	-4.327582	1.299075	-1.873832
H	-2.667109	0.881110	-2.419669
H	-3.337140	0.159909	-0.917215
C	-3.437353	2.414768	0.498266
H	-2.804790	3.044146	1.132892
H	-4.424138	2.886404	0.367060
H	-3.570675	1.443862	0.996087
C	-2.771335	5.049940	-0.643163
H	-2.953421	5.293042	0.415226
H	-2.590411	5.988005	-1.188081
H	-3.662626	4.570925	-1.062899
C	-0.325943	4.857435	-0.744024
H	-0.292410	5.475166	0.165108
H	0.488378	4.125763	-0.687080
H	-0.168911	5.515469	-1.613869
H	-0.063127	2.913266	-2.247762

Vibrational frequencies

-240.2089	18.6539	30.0797
31.3030	32.0707	40.6930
41.3011	44.9997	49.5722
56.7740	62.1162	68.2231
73.0227	82.4631	93.6786
105.9189	109.8288	114.8735
125.2992	129.3693	139.1686
149.8998	158.2323	162.8327
169.4028	180.1555	195.6081
198.0350	204.6706	208.3647

M7

Zero-point correction= 0.603255

Thermal correction to Energy= 0.637568

Thermal correction to Enthalpy= 0.638512

Thermal correction to Gibbs Free Energy= 0.539592

Sum of electronic and zero-point Energies= -1365.607744

Sum of electronic and thermal Energies= -1365.573431

Sum of electronic and thermal Enthalpies= -1365.572487
Sum of electronic and thermal Free Energies= -1365.671408

Cartesian coordinates

C	-2.365570	1.003249	-1.057923
H	-1.460400	1.619727	-0.961294
H	-2.800955	1.166745	-2.057628
H	-3.080763	1.356988	-0.302109
C	-0.914595	-0.824540	-1.881977
H	-0.040478	-0.167022	-1.787704
H	-0.574531	-1.866501	-1.754553
H	-1.311522	-0.723840	-2.906461
C	-1.374821	-0.637270	0.579265
H	-2.168012	-0.473719	1.316880
H	-1.091239	-1.705116	0.676848
C	-0.233199	0.235522	0.982085
C	-0.320913	1.361531	1.788367
O	0.598750	2.122887	2.153458
O	-1.626373	1.659309	2.186085
C	-1.758798	2.762652	3.034575
H	-1.383213	3.692584	2.575379
H	-2.832490	2.873931	3.245412
H	-1.218815	2.629725	3.988446
N	1.080799	-0.078716	0.505265
C	1.892255	0.892145	-0.088002
C	1.603942	-1.333259	0.781903
O	3.098436	0.935203	0.020452
O	1.213221	-2.045679	1.681575
O	1.160232	1.753492	-0.788431
O	2.491944	-1.697291	-0.148745
C	1.706978	3.007884	-1.261921
C	3.337076	-2.859935	0.013368
C	2.496764	-4.128554	-0.068286
H	3.151001	-5.013036	-0.049982
H	1.796279	-4.182426	0.773883
H	1.923371	-4.143100	-1.007764
C	4.113688	-2.767236	1.321014
H	3.443590	-2.851436	2.185530
H	4.857843	-3.575778	1.369390
H	4.641850	-1.803695	1.375432
C	4.283275	-2.764509	-1.174892
H	4.982523	-3.612982	-1.175420
H	3.715889	-2.776701	-2.117228

H	4.860633	-1.829481	-1.130540
C	2.339508	3.782091	-0.111553
H	3.300405	3.342458	0.182473
H	2.503173	4.826395	-0.417071
H	1.665854	3.744434	0.757088
C	2.689708	2.741170	-2.394914
H	3.056549	3.694038	-2.805277
H	3.544415	2.158468	-2.029027
H	2.198610	2.182445	-3.206320
C	0.477623	3.743749	-1.775321
H	0.766734	4.713773	-2.205111
H	-0.030884	3.152694	-2.551080
H	-0.232491	3.918724	-0.953957
C	-1.981846	-0.458955	-0.842192
C	-3.146411	-1.456408	-1.055535
H	-3.272976	-1.592448	-2.145578
H	-2.777149	-2.431927	-0.687521
C	-4.578253	-1.270706	-0.493482
C	-5.297932	-2.610413	-0.703372
H	-6.347688	-2.551343	-0.372785
H	-5.295625	-2.899400	-1.767061
H	-4.808435	-3.417573	-0.134950
C	-4.621419	-0.940376	1.000207
H	-4.082525	-1.695211	1.593559
H	-4.178234	0.040843	1.223024
H	-5.666622	-0.921827	1.351140
C	-5.361870	-0.203262	-1.267201
H	-4.961503	0.805825	-1.107921
H	-5.341697	-0.407471	-2.350086
H	-6.416913	-0.197541	-0.947362

Vibrational frequencies

27.8945	31.2907	37.5477
41.7994	52.5449	55.8175
62.5953	74.7168	83.6247
99.0029	107.2317	118.7891
124.1831	135.6147	148.6301
154.1699	162.4048	178.4151
187.6292	210.5696	220.8282
226.8228	229.1374	234.2668
241.0586	251.2299	260.3758
268.1840	271.0021	280.5686

M8

Zero-point correction= 0.806746
Thermal correction to Energy= 0.853270
Thermal correction to Enthalpy= 0.854215
Thermal correction to Gibbs Free Energy= 0.728079
Sum of electronic and zero-point Energies= -1727.854559
Sum of electronic and thermal Energies= -1727.808035
Sum of electronic and thermal Enthalpies= -1727.807091
Sum of electronic and thermal Free Energies= -1727.933226

Cartesian coordinates

C	1.245941	-2.854518	0.859721
H	0.421307	-2.487865	1.486788
H	1.319278	-3.947444	0.980257
H	2.170729	-2.398129	1.240170
C	-0.390381	-3.058421	-0.988438
H	-1.184667	-2.674471	-0.334224
H	-0.646146	-2.799464	-2.029873
H	-0.382919	-4.158393	-0.908468
C	0.899156	-0.924627	-0.728497
H	1.904398	-0.518262	-0.580801
H	0.641923	-0.706276	-1.783729
C	-0.005599	-0.168776	0.189203
C	0.380646	0.447465	1.366661
O	-0.349868	1.019523	2.206105
O	1.761789	0.414619	1.577663
C	2.201745	0.481854	2.905529
H	2.233821	-0.523317	3.366582
H	3.221206	0.895469	2.902958
H	1.546743	1.122653	3.513418
N	-1.401005	-0.078574	-0.124850
C	-2.388796	-0.388729	0.827906
C	-1.753364	0.512583	-1.318707
O	-3.436347	0.205284	0.933041
O	-0.985417	1.210704	-1.965770
O	-2.003446	-1.411972	1.575266
O	-2.958720	0.150753	-1.728061
C	-2.711198	-1.777294	2.790194
C	-3.637731	0.815457	-2.828362
C	-2.931294	0.498541	-4.139417
H	-3.510838	0.908200	-4.979869
H	-1.923909	0.931698	-4.155358
H	-2.852753	-0.590662	-4.274604

C	-3.718872	2.312220	-2.558914
H	-2.727581	2.780854	-2.601918
H	-4.364437	2.787364	-3.311730
H	-4.154239	2.491973	-1.564809
C	-5.023569	0.189887	-2.795332
H	-5.650193	0.611766	-3.593801
H	-4.956317	-0.898237	-2.940075
H	-5.506689	0.381617	-1.826499
C	-2.814451	-0.576416	3.721961
H	-3.547677	0.151323	3.353153
H	-3.121724	-0.915892	4.722239
H	-1.836071	-0.078054	3.779728
C	-4.071999	-2.359090	2.431571
H	-4.577589	-2.710199	3.343375
H	-4.701370	-1.602193	1.947060
H	-3.955463	-3.216019	1.750797
C	-1.813251	-2.842534	3.400460
H	-2.267331	-3.238841	4.319984
H	-1.664795	-3.673638	2.695733
H	-0.830077	-2.417165	3.647691
C	0.969594	-2.470558	-0.592321
C	1.998614	-3.037494	-1.600289
H	1.744410	-4.098998	-1.774331
H	1.787854	-2.533234	-2.561957
C	3.534504	-3.007812	-1.395750
C	4.153702	-3.395453	-2.745795
H	5.252364	-3.446799	-2.676316
H	3.791407	-4.380945	-3.080790
H	3.897243	-2.660774	-3.525981
C	4.084464	-1.634838	-1.002354
H	3.800194	-0.864396	-1.736404
H	3.725648	-1.311113	-0.014467
H	5.185772	-1.667260	-0.963338
C	3.994013	-4.045812	-0.364426
H	3.666065	-3.799101	0.653310
H	3.602880	-5.045937	-0.611829
H	5.094451	-4.110258	-0.353189
N	0.917812	3.562948	0.606939
C	1.856547	2.995935	-0.161434
N	3.165761	3.186144	0.119499
N	1.511722	2.269726	-1.216730
H	0.596164	1.793587	-1.293373
C	-0.468361	3.618962	0.185049

H	-0.915364	4.545039	0.574425
H	-0.538490	3.625061	-0.908291
H	-1.020710	2.755446	0.590067
C	1.122518	3.792250	2.025724
H	2.122526	3.465817	2.325731
H	0.992926	4.856228	2.277836
H	0.391899	3.173003	2.567800
C	3.678701	4.459895	0.579186
H	4.132966	4.383240	1.580200
H	4.449765	4.816618	-0.122972
H	2.876047	5.205430	0.609150
C	4.146205	2.196968	-0.271058
H	4.963869	2.201995	0.464097
H	3.690308	1.199307	-0.258641
H	4.584040	2.399012	-1.265225
H	2.220280	2.019759	-1.892066

Vibrational frequencies

16.8503	22.0177	31.9259
33.6743	38.2260	45.5583
46.5916	49.9050	58.4676
67.4447	70.6297	75.3577
76.1551	89.1636	93.8354
101.4477	103.5919	105.7774
117.7076	134.9988	136.2593
137.8471	151.8175	158.3245
167.8443	171.5108	178.7240
192.1889	202.2180	207.8558

TS5

Zero-point correction= 0.802408
Thermal correction to Energy= 0.848434
Thermal correction to Enthalpy= 0.849378
Thermal correction to Gibbs Free Energy= 0.723367
Sum of electronic and zero-point Energies= -1727.850701
Sum of electronic and thermal Energies= -1727.804674
Sum of electronic and thermal Enthalpies= -1727.803730
Sum of electronic and thermal Free Energies= -1727.929741

Cartesian coordinates

C	1.089524	-2.710320	1.218771
H	0.343848	-2.136461	1.783661
H	1.028215	-3.761227	1.543608

H	2.079499	-2.317665	1.485388
C	-0.631949	-3.061322	-0.534184
H	-1.359794	-2.472344	0.038429
H	-0.889851	-2.979974	-1.603416
H	-0.746006	-4.117958	-0.241003
C	0.934320	-1.108972	-0.739316
H	1.994729	-0.834210	-0.730865
H	0.631102	-1.072162	-1.800740
C	0.218614	0.018297	-0.025472
C	0.730229	0.581014	1.196591
O	0.125270	1.310028	1.975214
O	2.058270	0.344693	1.360097
C	2.678267	0.989296	2.451127
H	2.148627	0.783406	3.392626
H	3.700072	0.593431	2.503766
H	2.716279	2.080032	2.304111
N	-1.225635	0.081660	-0.131761
C	-2.087820	0.058303	0.983536
C	-1.765447	0.243480	-1.397250
O	-3.051759	0.777778	1.087226
O	-1.126649	0.629782	-2.351932
O	-1.708246	-0.855202	1.863654
O	-3.026249	-0.177450	-1.434904
C	-2.375702	-0.989645	3.153091
C	-3.885926	0.069239	-2.578822
C	-3.401694	-0.741041	-3.773853
H	-4.116390	-0.639671	-4.603996
H	-2.416119	-0.394547	-4.107794
H	-3.332974	-1.806568	-3.507252
C	-3.940822	1.562191	-2.874851
H	-2.976752	1.928997	-3.248561
H	-4.711251	1.759844	-3.634292
H	-4.203476	2.116993	-1.961664
C	-5.239198	-0.432423	-2.098859
H	-5.990724	-0.317467	-2.892802
H	-5.177767	-1.495957	-1.825252
H	-5.567411	0.135140	-1.216149
C	-2.354044	0.330159	3.913216
H	-3.021985	1.067888	3.453342
H	-2.679184	0.153094	4.949042
H	-1.334720	0.739559	3.917668
C	-3.789690	-1.507878	2.927420
H	-4.273920	-1.695793	3.897062

H	-4.388541	-0.777386	2.369192
H	-3.765530	-2.453942	2.365771
C	-1.532823	-2.028073	3.876460
H	-1.972699	-2.246100	4.860068
H	-1.486362	-2.962673	3.299126
H	-0.508095	-1.658394	4.026157
C	0.802292	-2.579436	-0.274670
C	1.717007	-3.462381	-1.161595
H	1.323263	-4.493701	-1.115701
H	1.536825	-3.135220	-2.202184
C	3.251232	-3.595813	-0.981908
C	3.764380	-4.313161	-2.238381
H	4.848892	-4.497234	-2.172459
H	3.265209	-5.286628	-2.371783
H	3.576773	-3.712489	-3.142803
C	3.990351	-2.259727	-0.868022
H	3.791401	-1.614172	-1.737987
H	3.710903	-1.703638	0.038673
H	5.077763	-2.436335	-0.828349
C	3.611268	-4.471294	0.225209
H	3.360717	-3.994085	1.181101
H	3.083811	-5.437906	0.181980
H	4.693332	-4.680942	0.232871
N	0.798050	3.751747	-0.089390
C	1.808518	3.055888	-0.671367
N	3.083375	3.515987	-0.496896
N	1.530276	1.971083	-1.353649
H	0.776459	1.095991	-0.799407
C	-0.572008	3.507057	-0.485516
H	-1.127681	4.457548	-0.466611
H	-0.595501	3.082311	-1.495404
H	-1.062857	2.797171	0.201200
C	0.946402	4.395835	1.198040
H	1.994251	4.391152	1.516045
H	0.590268	5.437848	1.163732
H	0.361395	3.836500	1.946588
C	3.399164	4.927988	-0.540573
H	3.916703	5.260729	0.374246
H	4.055832	5.139286	-1.401820
H	2.482579	5.516677	-0.661629
C	4.194873	2.613137	-0.680952
H	5.036381	2.948685	-0.057036
H	3.912541	1.601656	-0.358622

H 4.546357 2.574414 -1.729140
H 2.298094 1.611748 -1.910916

Vibrational frequencies
-1335.7095 17.2428 21.5436
23.7938 26.8374 31.8536
35.8166 39.3888 49.7886
55.9400 62.6232 69.4712
75.2640 84.0186 85.6395
99.1213 105.5000 109.9189
119.9498 126.1682 134.0461
137.9606 147.0543 155.4624
157.0740 160.6796 176.3920
178.1902 192.8150 206.2173

P1
Zero-point correction= 0.617435
Thermal correction to Energy= 0.652364
Thermal correction to Enthalpy= 0.653308
Thermal correction to Gibbs Free Energy= 0.551091
Sum of electronic and zero-point Energies= -1366.118047
Sum of electronic and thermal Energies= -1366.083118
Sum of electronic and thermal Enthalpies= -1366.082174
Sum of electronic and thermal Free Energies= -1366.184390

Cartesian coordinates
C -1.176383 -1.980248 0.326050
C -0.425858 -2.021487 -1.014906
H 0.657283 -1.901930 -0.880074
H -0.584492 -2.992504 -1.510031
H -0.754630 -1.235390 -1.706501
C -0.429368 -2.882579 1.316828
H 0.620196 -2.578595 1.443550
H -0.908881 -2.867311 2.309061
H -0.428705 -3.925589 0.962463
C -1.293379 -0.554481 0.889764
H -1.784104 0.087917 0.151305
H -1.953914 -0.589983 1.767785
C -0.019375 0.147973 1.366817
C -0.274905 1.516135 1.985515
O 0.507529 2.432394 1.952085
O -1.443217 1.568243 2.613910
C -1.752081 2.787151 3.277080

H	-1.825412	3.611641	2.553451
H	-2.717838	2.631064	3.769592
H	-0.979511	3.032039	4.019168
N	1.057064	0.267610	0.389798
C	0.970065	1.201652	-0.651557
C	2.235939	-0.435878	0.671977
O	1.894877	1.594130	-1.313745
O	2.480919	-0.852696	1.782310
O	-0.293400	1.593345	-0.770457
O	2.952660	-0.639363	-0.409789
C	-0.688239	2.702870	-1.631839
C	4.283908	-1.241002	-0.362434
C	4.181868	-2.679476	0.123390
H	5.162795	-3.167095	0.024744
H	3.869230	-2.722961	1.173727
H	3.458204	-3.238586	-0.488619
C	5.194742	-0.391608	0.511280
H	4.878946	-0.417487	1.561807
H	6.223295	-0.774623	0.445786
H	5.191327	0.651498	0.161857
C	4.722014	-1.188074	-1.816804
H	5.732706	-1.606900	-1.921404
H	4.034187	-1.770163	-2.447237
H	4.729889	-0.149560	-2.176837
C	0.062735	3.964294	-1.229474
H	1.132551	3.880462	-1.456446
H	-0.348561	4.822383	-1.780463
H	-0.056167	4.148445	-0.152017
C	-0.455844	2.321432	-3.086118
H	-0.849773	3.112329	-3.740876
H	0.613857	2.191830	-3.291688
H	-0.981614	1.384461	-3.324147
C	-2.173246	2.845419	-1.336660
H	-2.597361	3.666088	-1.932053
H	-2.712039	1.920232	-1.587915
H	-2.336072	3.065758	-0.271465
C	-2.593363	-2.596537	0.184820
H	-2.438437	-3.582017	-0.288440
H	-2.954726	-2.818767	1.204974
C	-4.828797	-3.027299	-0.748769
H	-5.737810	-2.625073	-1.223442
H	-4.440451	-3.835134	-1.389115
H	-5.120942	-3.472596	0.215930

C	-3.779923	-1.923075	-0.552013
C	-4.439227	-0.814618	0.280151
H	-4.687009	-1.173848	1.291906
H	-3.805639	0.075424	0.386222
H	-5.378135	-0.492861	-0.198632
C	-3.413293	-1.365724	-1.929372
H	-2.732484	-0.504845	-1.859258
H	-2.932151	-2.128161	-2.560903
H	-4.322067	-1.023494	-2.450387
H	0.422118	-0.436811	2.189165

Vibrational frequencies

22.0886	24.5328	29.0924
31.4233	35.1562	46.9008
51.4243	60.1371	67.5885
77.7364	97.5077	106.2469
124.2747	127.7375	133.8079
142.2759	149.0201	170.2884
191.9874	203.6291	214.0882
217.1645	219.2144	224.2408
234.3358	240.2627	257.7161
260.9972	264.9360	267.3570

Ra

Zero-point correction= 0.348536
Thermal correction to Energy= 0.365448
Thermal correction to Enthalpy= 0.366392
Thermal correction to Gibbs Free Energy= 0.304094
Sum of electronic and zero-point Energies= -638.659357
Sum of electronic and thermal Energies= -638.642446
Sum of electronic and thermal Enthalpies= -638.641501
Sum of electronic and thermal Free Energies= -638.703799

Cartesian coordinates

C	-1.096799	0.667613	0.479862
C	-1.510817	0.677099	1.953804
H	-1.457175	-0.333186	2.383321
H	-0.825924	1.325673	2.521505
H	-2.529593	1.067085	2.084712
C	-1.225902	2.079749	-0.091557
H	-0.564919	2.779779	0.443569
H	-0.971577	2.115440	-1.161964
H	-2.251291	2.451465	0.015698

C	-3.397225	-0.545515	-0.385934
N	0.274449	0.149995	0.480742
C	1.232562	0.754562	-0.088840
H	1.112393	1.717435	-0.617618
C	2.604675	0.216344	-0.095785
C	2.913780	-0.998406	0.534325
C	3.622370	0.926752	-0.744446
C	4.214038	-1.488905	0.513118
C	4.926768	0.434794	-0.765926
C	5.224499	-0.773695	-0.137372
H	4.447440	-2.436036	1.005838
H	5.713478	0.996402	-1.275253
C	-1.859130	-0.378130	-0.375661
H	-1.435737	-1.358899	-0.102208
H	-1.533635	-0.199594	-1.415596
C	-3.702290	-1.473745	-1.570280
H	-4.779152	-1.699564	-1.623346
H	-3.405056	-1.011428	-2.524994
H	-3.161046	-2.428791	-1.475463
C	-3.909720	-1.233891	0.884556
H	-3.363973	-2.172315	1.072405
H	-3.810747	-0.602743	1.777085
H	-4.977472	-1.483386	0.775630
C	-4.162050	0.762278	-0.597967
H	-4.083411	1.434616	0.269134
H	-3.799975	1.303525	-1.485949
H	-5.232829	0.550691	-0.748524
H	2.108941	-1.540214	1.035486
H	6.245991	-1.161562	-0.152810
H	3.385566	1.874225	-1.237251

Vibrational frequencies

22.5230	43.8015	49.5190
93.9323	101.8740	140.5415
199.6102	225.8877	244.7786
269.2541	275.9002	282.0177
284.9625	307.1544	317.6121
325.3755	333.3847	367.3087
378.2586	391.0842	420.5297
429.6998	440.5474	487.3258
516.5519	543.9859	568.6830
629.3219	657.4684	720.1610

^{2}Sa

Zero-point correction= 0.347518
Thermal correction to Energy= 0.364977
Thermal correction to Enthalpy= 0.365921
Thermal correction to Gibbs Free Energy= 0.300692
Sum of electronic and zero-point Energies= -638.428295
Sum of electronic and thermal Energies= -638.410836
Sum of electronic and thermal Enthalpies= -638.409892
Sum of electronic and thermal Free Energies= -638.475121

Cartesian coordinates

C	-1.146877	0.809599	0.418537
C	-1.398914	0.686285	1.924423
H	-1.193962	-0.332574	2.277664
H	-0.759215	1.391144	2.473193
H	-2.445186	0.933896	2.139760
C	-1.451364	2.253276	-0.056172
H	-0.867370	2.983477	0.520612
H	-1.243506	2.370693	-1.128372
H	-2.516584	2.442586	0.120629
C	-3.299560	-0.657521	-0.348644
N	0.254303	0.660716	0.211787
C	1.354862	1.033070	-0.261941
H	1.349767	2.001455	-0.800966
C	2.611584	0.314394	-0.157895
C	2.693173	-0.910468	0.528830
C	3.750641	0.872134	-0.759345
C	3.911171	-1.567367	0.607318
C	4.966995	0.204283	-0.674544
C	5.045766	-1.010776	0.006331
H	3.983901	-2.517894	1.139074
H	5.856623	0.632299	-1.140010
C	-1.804322	-0.280276	-0.470233
H	-1.228225	-1.206858	-0.314836
H	-1.610063	0.026740	-1.510837
C	-3.584626	-1.541848	-1.571282
H	-4.623233	-1.905381	-1.546893
H	-3.442211	-0.984264	-2.510130
H	-2.920485	-2.420329	-1.593522
C	-3.588058	-1.488071	0.906823
H	-2.902460	-2.346746	0.982606
H	-3.508115	-0.905648	1.833648
H	-4.614249	-1.884131	0.862005

C	-4.240381	0.547565	-0.397531
H	-4.172282	1.170549	0.506942
H	-4.043775	1.182426	-1.275276
H	-5.282741	0.200362	-0.466036
H	1.801749	-1.333468	0.998012
H	6.002794	-1.533107	0.072269
H	3.678169	1.824092	-1.290096

Vibrational frequencies

17.0410	25.9515	35.4958
60.3102	107.9743	132.1522
181.9975	218.8707	230.8685
245.0342	252.9013	263.5159
275.7250	281.2377	310.8969
315.0120	331.0480	356.4135
377.8534	388.2709	415.1414
425.0546	430.4618	465.8223
477.1287	516.0011	552.3618
624.7734	638.1576	704.7714

^{3}M3b

Zero-point correction= 0.332127
Thermal correction to Energy= 0.349365
Thermal correction to Enthalpy= 0.350309
Thermal correction to Gibbs Free Energy= 0.286327
Sum of electronic and zero-point Energies= -638.078064
Sum of electronic and thermal Energies= -638.060826
Sum of electronic and thermal Enthalpies= -638.059882
Sum of electronic and thermal Free Energies= -638.123864

Cartesian coordinates

C	-1.154983	0.930735	-0.348515
C	-1.761797	2.190364	0.270446
H	-1.716835	2.146037	1.369202
H	-1.176510	3.064806	-0.053283
H	-2.807585	2.342526	-0.034407
C	-1.281547	1.009907	-1.876548
H	-0.713817	1.880169	-2.241876
H	-0.844267	0.109693	-2.334774
H	-2.320876	1.112811	-2.217000
N	0.254414	0.932614	0.015485
C	1.119162	0.089526	-0.416303
C	2.489743	-0.084519	-0.152392

C	3.206604	0.771492	0.768618
C	3.269114	-1.115764	-0.783226
C	4.555841	0.598006	1.012161
C	4.616325	-1.272572	-0.525068
C	5.298309	-0.420520	0.377249
H	5.059973	1.269201	1.717699
H	5.166487	-2.073641	-1.031206
C	-1.762409	-0.377991	0.224238
H	-1.356594	-0.464170	1.247212
H	-1.275528	-1.189083	-0.345735
C	-4.031586	-0.484633	-0.993679
H	-4.104179	0.580638	-1.258173
H	-3.545548	-1.010476	-1.830413
H	-5.060293	-0.871420	-0.905897
C	-3.365537	-2.189048	0.680426
H	-2.819507	-2.402849	1.613417
H	-4.414092	-2.497375	0.823935
H	-2.931969	-2.818399	-0.113175
C	-3.273402	-0.700230	0.317458
C	-3.964681	0.089645	1.434961
H	-3.436282	-0.039907	2.393169
H	-4.012321	1.165564	1.221374
H	-4.999054	-0.266597	1.571471
H	2.643391	1.563231	1.270935
H	6.364922	-0.548239	0.576403
H	2.764652	-1.787210	-1.486238

Vibrational frequencies

28.6819	36.9535	48.2239
71.1103	125.1457	133.4251
180.1327	210.6020	237.7117
245.5843	265.2151	275.7874
303.3039	307.5763	313.5950
323.4014	326.0549	360.2061
379.1724	392.4536	430.3358
431.8658	434.0481	480.7045
495.3260	508.5238	551.1638
622.6993	628.9695	660.7231

^{3}Ea

Zero-point correction= 0.345333

Thermal correction to Energy= 0.362546

Thermal correction to Enthalpy= 0.363491

Thermal correction to Gibbs Free Energy= 0.299866

Sum of electronic and zero-point Energies= -638.580898
Sum of electronic and thermal Energies= -638.563685
Sum of electronic and thermal Enthalpies= -638.562741
Sum of electronic and thermal Free Energies= -638.626365

Cartesian coordinates

C	1.281943	-1.265223	0.253770
C	1.975039	-1.453790	1.600301
H	1.530664	-0.804163	2.368320
H	1.857730	-2.497753	1.925460
H	3.048615	-1.231880	1.533610
C	1.938298	-2.178727	-0.799698
H	1.828611	-3.233046	-0.505474
H	1.472808	-2.038607	-1.786362
H	3.009183	-1.957693	-0.886355
C	2.371479	1.185372	-0.234523
N	-0.067606	-1.810515	0.405995
C	-1.081412	-1.539760	-0.462402
H	-1.127789	-2.167606	-1.363821
C	-2.141894	-0.637423	-0.189575
C	-2.209414	0.097981	1.026017
C	-3.182235	-0.441468	-1.137784
C	-3.246468	0.989061	1.260142
C	-4.211226	0.453355	-0.890261
C	-4.254166	1.180697	0.307144
H	-3.277477	1.541550	2.203033
H	-4.996459	0.590901	-1.638364
C	1.176979	0.203069	-0.220041
H	0.392822	0.682277	0.388861
H	0.763207	0.161242	-1.241775
C	1.888061	2.407170	-1.029142
H	2.660964	3.191753	-1.047964
H	1.652743	2.137360	-2.070936
H	0.979202	2.838909	-0.580080
C	2.743706	1.666531	1.172518
H	1.860437	2.056508	1.703146
H	3.185153	0.872898	1.789161
H	3.482606	2.481228	1.108777
C	3.615049	0.625609	-0.927337
H	4.079796	-0.187960	-0.350800
H	3.380376	0.243924	-1.933300
H	4.372838	1.417517	-1.038665
H	-3.157674	-1.002548	-2.075876

H	-5.067807	1.884124	0.497073
H	-1.439734	-0.060057	1.785587

Vibrational frequencies

24.1250	40.9105	52.4488
81.2114	128.1595	145.6634
179.7222	217.3518	246.6398
248.1939	267.4588	274.9723
289.7920	298.5517	316.9019
325.8875	328.8681	363.7199
381.6930	403.6861	422.2471
426.6356	435.3473	461.4018
510.6690	532.0974	549.7059
605.2283	625.3465	680.5430

^{3}Eb

Zero-point correction= 0.534822
Thermal correction to Energy= 0.564284
Thermal correction to Enthalpy= 0.565228
Thermal correction to Gibbs Free Energy= 0.470403
Sum of electronic and zero-point Energies= -1000.329737
Sum of electronic and thermal Energies= -1000.300275
Sum of electronic and thermal Enthalpies= -1000.299331
Sum of electronic and thermal Free Energies= -1000.394157

Cartesian coordinates

C	2.219548	-0.791808	1.437001
C	3.536089	-0.917755	2.198197
H	4.253514	-0.148449	1.876584
H	3.348889	-0.782735	3.273578
H	3.993693	-1.905470	2.049377
C	1.249613	-1.898057	1.895047
H	1.046295	-1.791904	2.970948
H	0.293722	-1.833084	1.355538
H	1.683626	-2.890719	1.725081
C	3.175402	-1.743668	-0.937758
N	1.583954	0.442932	1.901242
C	0.573543	1.042834	1.216631
H	-0.440719	0.610877	1.327021
C	0.726354	2.221361	0.443742
C	1.980289	2.876757	0.288820
C	-0.402163	2.791893	-0.210070
C	2.093033	4.018342	-0.491326

C	-0.271808	3.931348	-0.987643
C	0.974695	4.556057	-1.141308
H	3.066919	4.504895	-0.594638
H	-1.152299	4.347274	-1.485205
C	2.373375	-0.722408	-0.098999
H	2.796152	0.269724	-0.330319
H	1.347140	-0.695701	-0.499843
C	2.816520	-1.443826	-2.400245
H	3.384289	-2.093996	-3.084602
H	1.743285	-1.608311	-2.587235
H	3.045591	-0.397611	-2.658881
C	4.689261	-1.560960	-0.783359
H	4.982367	-0.516127	-0.974064
H	5.048299	-1.834083	0.217518
H	5.223147	-2.196042	-1.508389
C	2.805280	-3.199046	-0.645555
H	3.136543	-3.519609	0.353353
H	1.717909	-3.359820	-0.714787
H	3.289735	-3.865135	-1.377340
H	-1.373889	2.305497	-0.087636
H	1.071213	5.454540	-1.754952
H	2.855469	2.475214	0.806108
N	-4.730391	-0.520059	0.335694
C	-3.351395	-0.489870	0.198800
N	-2.866767	-1.163389	-0.904754
N	-2.538393	0.091522	1.016810
H	-3.046838	0.697212	1.660386
C	-5.301294	-0.145056	1.602912
H	-6.315027	-0.565420	1.682707
H	-4.697583	-0.550948	2.426627
H	-5.383273	0.952644	1.735372
C	-5.590837	-0.301031	-0.807347
H	-5.018530	-0.407112	-1.735740
H	-6.427545	-1.019105	-0.824107
H	-6.018183	0.719008	-0.787150
C	-3.405617	-2.452995	-1.277300
H	-3.545758	-2.527366	-2.368377
H	-2.722394	-3.266221	-0.967346
H	-4.370970	-2.620362	-0.786790
C	-1.489303	-0.965230	-1.273601
H	-1.361754	-1.200061	-2.341805
H	-1.193157	0.075112	-1.095461
H	-0.802211	-1.614929	-0.698296

Vibrational frequencies

4.9260	22.1633	25.4523
35.6785	40.1672	41.2575
54.4544	61.3802	72.9672
88.2776	97.5270	105.4038
122.8320	130.7441	138.7346
146.0613	179.4307	197.4883
216.0519	219.3801	236.5494
239.7791	246.0834	264.8699
278.1883	279.5760	287.2918
306.1441	306.6836	309.5371

TSa

Zero-point correction= 1.241995
Thermal correction to Energy= 1.328627
Thermal correction to Enthalpy= 1.329571
Thermal correction to Gibbs Free Energy= 1.115133
Sum of electronic and zero-point Energies= -4876.939632
Sum of electronic and thermal Energies= -4876.853000
Sum of electronic and thermal Enthalpies= -4876.852056
Sum of electronic and thermal Free Energies= -4877.066494

Cartesian coordinates

Ir	-2.492590	0.571104	-0.175676
C	-3.969950	-3.863814	0.990973
C	-3.128591	-3.703746	-0.103915
C	-2.681161	-2.438950	-0.427470
C	-4.015895	-1.475401	1.260743
C	-4.402850	-2.741886	1.673826
H	-4.281959	-4.857786	1.306347
H	-1.991498	-2.279194	-1.246687
H	-5.075185	-2.850758	2.524895
C	-4.481236	2.211040	1.456045
C	-3.995411	0.970266	1.093623
C	-4.499712	-0.196346	1.748668
C	-5.460087	-0.039418	2.766521
C	-5.936438	1.207480	3.128994
C	-5.437832	2.315465	2.457233
H	-4.136327	3.126523	0.967647
H	-6.683670	1.308032	3.925625
N	-3.093715	-1.346343	0.226761
F	-5.944464	-1.099137	3.402422

F	-5.890023	3.521237	2.797718
C	-2.795470	-4.885978	-0.975196
F	-1.894031	-4.577979	-1.912794
F	-3.894879	-5.304787	-1.616753
F	-2.339292	-5.926872	-0.296448
C	1.152231	-1.947053	-2.181084
C	0.212818	-1.344324	-3.024520
C	-0.707410	-0.449571	-2.510638
C	0.225042	-0.614424	-0.391450
C	1.177815	-1.516223	-0.849897
H	0.181429	-1.575685	-4.090600
H	-1.491017	-0.010131	-3.130102
C	0.961711	-0.029606	3.299248
C	1.159946	-0.373331	1.965413
C	0.127833	-0.189050	1.022798
C	-1.236447	0.746573	2.658333
C	-0.270059	0.551812	3.640664
H	2.108475	-0.781297	1.610021
H	-2.206384	1.192388	2.890000
H	-0.494527	0.851210	4.646540
N	-0.751248	-0.152476	-1.194227
N	-1.040903	0.370065	1.394062
C	-4.432470	2.443433	-3.430027
C	-5.256389	1.507673	-4.022988
C	-5.294610	0.223804	-3.453838
C	-4.547248	-0.108432	-2.329045
C	-3.700453	0.828595	-1.746255
C	-3.653870	2.133920	-2.312073
H	-5.841911	1.757203	-4.907428
H	-4.636263	-1.131052	-1.945191
C	-1.655352	5.180535	-1.208647
C	-2.553078	4.417661	-1.945077
C	-2.750334	3.073369	-1.621118
C	-1.210358	3.245633	0.124100
C	-0.952306	4.584096	-0.146352
H	-1.476698	6.224840	-1.458629
H	-3.080547	4.871460	-2.771990
H	-0.685609	2.735219	0.950993
F	-6.094371	-0.666962	-4.010446
F	-4.388095	3.654912	-3.977487
N	-2.078290	2.530692	-0.577876
C	0.049528	5.354446	0.659003
F	-0.545204	6.374654	1.332763

F	0.992565	5.914173	-0.154554
F	0.673354	4.557056	1.555597
C	1.977143	-0.322632	4.392872
C	3.204505	-1.036003	3.817145
H	3.709511	-0.420455	3.073725
H	3.937210	-1.243919	4.632178
H	2.938106	-2.004205	3.371047
C	2.409292	0.994543	5.053830
H	3.132656	0.797167	5.852331
H	2.883721	1.692569	4.320257
H	1.546909	1.523032	5.517405
C	1.299981	-1.230037	5.449229
H	0.486662	-0.698383	5.972628
H	0.874884	-2.138904	4.985656
H	2.046206	-1.537654	6.190493
H	1.880748	-1.944264	-0.129770
C	2.033471	-3.085535	-2.695656
C	1.094484	-4.229966	-3.126962
H	0.385027	-3.924339	-3.923640
H	1.701385	-5.067556	-3.523539
H	0.503171	-4.593703	-2.261102
C	2.871720	-2.620306	-3.908128
H	3.634799	-1.878503	-3.568052
H	3.416670	-3.489326	-4.325902
H	2.263410	-2.167411	-4.713623
C	2.968563	-3.618822	-1.611409
H	3.659185	-2.827874	-1.270694
H	2.407214	-3.996295	-0.757225
H	3.568820	-4.448441	-2.006554
P	0.336846	-4.304171	1.798104
F	0.111875	-4.449190	0.180812
F	1.184238	-5.697147	1.818536
F	1.727936	-3.456500	1.511069
F	0.579510	-4.106613	3.408422
F	-0.516181	-2.878963	1.774384
F	-1.022242	-5.123578	2.099294
C	4.757850	2.486641	0.949568
C	4.599601	2.561757	2.458339
H	3.568215	2.852389	2.717622
H	4.790859	1.574741	2.895794
H	5.280359	3.280371	2.913643
C	6.186071	2.031503	0.605359
H	6.368709	1.008843	0.999791

H	6.357099	2.002964	-0.488226
H	6.940350	2.710803	1.040796
C	4.916202	5.216994	0.611590
N	3.813983	1.468357	0.467430
C	3.728775	1.036485	-0.758288
C	2.816510	1.381505	-1.782804
C	1.722467	2.303124	-1.581314
C	2.930910	0.837883	-3.100284
C	0.857994	2.649114	-2.599799
C	2.051275	1.195263	-4.119373
C	1.018115	2.105127	-3.887135
H	0.056791	3.371145	-2.402534
H	2.187866	0.760949	-5.121413
C	4.383564	3.796141	0.199272
H	3.284795	3.884357	0.223226
H	4.638446	3.627222	-0.865046
C	4.593170	6.125242	-0.585689
H	4.840952	7.167404	-0.361149
H	5.180683	5.830915	-1.480572
H	3.512676	6.075871	-0.851441
C	4.173914	5.755972	1.847283
H	3.077640	5.757654	1.675197
H	4.384111	5.180168	2.761162
H	4.487751	6.808091	2.021874
C	6.436248	5.265841	0.847291
H	6.733959	4.710933	1.767019
H	6.994310	4.847752	-0.004268
H	6.755961	6.294922	0.989519
H	4.769607	-0.026070	-1.144811
N	7.186489	-2.418123	-1.903765
C	6.225251	-1.805537	-1.158185
N	5.801603	-2.438735	-0.037924
N	5.672014	-0.685964	-1.574033
H	6.204425	-0.172450	-2.266518
C	7.297695	-2.121575	-3.330806
H	7.738260	-3.010737	-3.837807
H	6.301321	-1.947481	-3.743064
H	7.944188	-1.246172	-3.524574
C	8.377011	-2.981566	-1.306053
H	8.322356	-2.916281	-0.202722
H	8.507209	-4.052491	-1.579853
H	9.267935	-2.427670	-1.627358
C	5.931940	-3.877519	0.150379

H	6.705876	-4.120721	0.891098
H	4.967103	-4.272885	0.506338
H	6.184453	-4.357491	-0.804738
C	5.068658	-1.756376	1.004115
H	5.621027	-1.844514	1.966590
H	4.900982	-0.678150	0.771996
H	4.088197	-2.237792	1.147085
H	3.724229	0.122917	-3.309952
H	1.598332	2.709180	-0.564388
H	0.323640	2.392264	-4.681609

Vibrational frequencies

-677.9270	2.8076	14.3218
18.1529	19.8598	22.5491
26.1235	29.5144	30.4358
32.4071	34.9103	36.2571
36.9567	38.5743	42.4525
43.6661	49.9672	51.6735
59.0011	60.8640	62.6953
68.8670	71.8286	71.9343
75.7362	77.8085	81.5623
82.0056	84.1964	86.9901

SET1

M1-B1

0 1

C	2.39546100	0.31110100	-0.73182800
C	2.87610700	-0.38564900	-2.00794900
H	2.81166600	-1.47799300	-1.90352500
H	2.23196400	-0.08763600	-2.84977800
H	3.91024400	-0.11082900	-2.25977000
C	2.53599400	1.82491100	-0.90612800
H	1.90731200	2.18318000	-1.73669200
H	2.24808900	2.37457200	0.00310300
H	3.57231500	2.09463400	-1.13982700
C	4.64069300	-0.32315400	0.71208000
N	1.01827900	-0.15799200	-0.54696600
C	0.06331700	0.66862600	-0.38060200
H	0.23323800	1.75566500	-0.37783700
C	-1.34576500	0.32626300	-0.17231000
C	-1.87591600	-0.98635500	-0.16682300
C	-2.26195700	1.39246600	0.04134800
C	-3.24212600	-1.22350600	0.04484900

C	-3.61918300	1.16733600	0.25082900
C	-4.10351700	-0.14528200	0.25258300
H	-3.62284800	-2.24063200	0.04532600
H	-4.32633000	1.97734500	0.41668400
O	-1.73757400	2.63253300	0.03156800
O	-1.01790000	-1.99092900	-0.37525400
O	-5.42388100	-0.27956800	0.46326700
C	-1.48022300	-3.31655200	-0.38121500
H	-0.60248000	-3.94727800	-0.56833500
H	-1.92391200	-3.60029700	0.58804700
H	-2.22153300	-3.48952500	-1.17966800
C	-2.57687300	3.74132400	0.23326500
H	-3.06548100	3.70624200	1.22116900
H	-1.93553700	4.62953500	0.18255100
H	-3.35165200	3.81171700	-0.54823200
C	-5.98798800	-1.56781200	0.48125400
H	-5.55908200	-2.18820400	1.28592200
H	-7.06097000	-1.43643400	0.66610900
H	-5.85122400	-2.08527900	-0.48307900
C	3.10753500	-0.18818100	0.55366200
H	2.67568700	-1.17990000	0.76798500
H	2.74306000	0.46893200	1.36304600
C	4.88471500	-0.55585500	2.20988300
H	5.95473100	-0.72368700	2.41177400
H	4.55900800	0.31188400	2.80546200
H	4.33050300	-1.43777800	2.56925700
C	5.19107800	-1.54055500	-0.04025100
H	4.63912800	-2.45429700	0.23215800
H	5.13300000	-1.42482300	-1.13029100
H	6.25060800	-1.69929200	0.21821300
C	5.41993200	0.92486600	0.29219600
H	5.38310100	1.08961400	-0.79478900
H	5.03541900	1.82931700	0.78905200
H	6.48114900	0.81695900	0.56902700

1 2

C	2.39546100	0.31110100	-0.73182800
C	2.87610700	-0.38564900	-2.00794900
H	2.81166600	-1.47799300	-1.90352500
H	2.23196400	-0.08763600	-2.84977800
H	3.91024400	-0.11082900	-2.25977000
C	2.53599400	1.82491100	-0.90612800
H	1.90731200	2.18318000	-1.73669200
H	2.24808900	2.37457200	0.00310300

H	3.57231500	2.09463400	-1.13982700
C	4.64069300	-0.32315400	0.71208000
N	1.01827900	-0.15799200	-0.54696600
C	0.06331700	0.66862600	-0.38060200
H	0.23323800	1.75566500	-0.37783700
C	-1.34576500	0.32626300	-0.17231000
C	-1.87591600	-0.98635500	-0.16682300
C	-2.26195700	1.39246600	0.04134800
C	-3.24212600	-1.22350600	0.04484900
C	-3.61918300	1.16733600	0.25082900
C	-4.10351700	-0.14528200	0.25258300
H	-3.62284800	-2.24063200	0.04532600
H	-4.32633000	1.97734500	0.41668400
O	-1.73757400	2.63253300	0.03156800
O	-1.01790000	-1.99092900	-0.37525400
O	-5.42388100	-0.27956800	0.46326700
C	-1.48022300	-3.31655200	-0.38121500
H	-0.60248000	-3.94727800	-0.56833500
H	-1.92391200	-3.60029700	0.58804700
H	-2.22153300	-3.48952500	-1.17966800
C	-2.57687300	3.74132400	0.23326500
H	-3.06548100	3.70624200	1.22116900
H	-1.93553700	4.62953500	0.18255100
H	-3.35165200	3.81171700	-0.54823200
C	-5.98798800	-1.56781200	0.48125400
H	-5.55908200	-2.18820400	1.28592200
H	-7.06097000	-1.43643400	0.66610900
H	-5.85122400	-2.08527900	-0.48307900
C	3.10753500	-0.18818100	0.55366200
H	2.67568700	-1.17990000	0.76798500
H	2.74306000	0.46893200	1.36304600
C	4.88471500	-0.55585500	2.20988300
H	5.95473100	-0.72368700	2.41177400
H	4.55900800	0.31188400	2.80546200
H	4.33050300	-1.43777800	2.56925700
C	5.19107800	-1.54055500	-0.04025100
H	4.63912800	-2.45429700	0.23215800
H	5.13300000	-1.42482300	-1.13029100
H	6.25060800	-1.69929200	0.21821300
C	5.41993200	0.92486600	0.29219600
H	5.38310100	1.08961400	-0.79478900
H	5.03541900	1.82931700	0.78905200
H	6.48114900	0.81695900	0.56902700

Ir(III)*-Ir(II)

0 3

Ir	1.40318200	-0.37401300	-0.05211600
C	-0.83621300	-4.32254200	-1.66326200
C	-1.42325800	-3.58895800	-0.60636400
C	-0.80612500	-2.43002300	-0.17584200
C	0.92035700	-2.66529800	-1.77116200
C	0.32345900	-3.85285000	-2.23969600
H	-1.29516200	-5.24572700	-2.02092400
H	-1.23392000	-1.83910300	0.63346000
H	0.78848400	-4.39373200	-3.06024400
C	3.60478700	-0.06766700	-2.08876000
C	2.49998200	-0.80157100	-1.62365900
C	2.09553300	-2.01870600	-2.28646600
C	2.88512200	-2.45170800	-3.36931700
C	3.97132200	-1.73130600	-3.82551300
C	4.31557700	-0.53517100	-3.17555600
H	3.92221700	0.85650400	-1.60471600
H	4.54938600	-2.09222400	-4.67701800
N	0.33647300	-1.98930700	-0.71358300
F	2.59013300	-3.58864900	-4.00060800
F	5.36387400	0.14568600	-3.63227700
C	-2.65984300	-4.09853100	0.06319600
F	-3.09760200	-3.28073300	1.01799800
F	-2.43208200	-5.29331600	0.63928700
F	-3.65252900	-4.28943300	-0.81040100
C	-2.09305600	1.09710400	3.18093000
C	-1.03065800	0.28598200	3.60558600
C	-0.04906400	-0.09586500	2.70892700
C	-1.06482600	1.07420000	0.98787300
C	-2.07131500	1.50583000	1.84824400
H	-0.96391600	-0.07423600	4.63264300
H	0.77890800	-0.73891000	3.01303500
C	-1.94722100	2.44650300	-2.43791500
C	-2.00613600	2.19029700	-1.06827900
C	-1.03373000	1.41025300	-0.44771800
C	0.07077600	1.12269000	-2.46202800
C	-0.86524200	1.88877600	-3.13348900
H	-2.83948700	2.56203400	-0.48055200
H	0.92004800	0.67759100	-2.98352900
H	-0.74099100	2.03755400	-4.20675500
N	-0.07403100	0.27505400	1.42216300

N	-0.00767100	0.89009300	-1.14571000
C	4.45031300	-1.31357400	2.66957400
C	4.29794600	-2.65101300	2.98754500
C	3.23564000	-3.35948100	2.41608600
C	2.34641900	-2.76344800	1.53945900
C	2.50583200	-1.40710400	1.21804500
C	3.56864500	-0.63987300	1.80627300
H	4.99543700	-3.13663800	3.67069400
H	1.54307700	-3.36409700	1.11142800
C	4.38231700	3.05029600	1.56931200
C	4.52216200	1.72680500	1.93175000
C	3.61206300	0.76067000	1.46329800
C	2.45284900	2.43580100	0.27353800
C	3.31036600	3.41891700	0.72617100
H	5.08880400	3.79863900	1.93236400
H	5.33265300	1.41947100	2.58798600
H	1.62827400	2.67690200	-0.39811700
F	3.09398500	-4.64415900	2.73153600
F	5.47571900	-0.66385800	3.22175000
N	2.60023200	1.14954800	0.60903300
C	3.11514500	4.84666300	0.32801900
F	4.20379400	5.34239900	-0.27396600
F	2.88136800	5.62591200	1.39223500
F	2.08768500	4.99993100	-0.51200400
C	-2.99550000	3.27650600	-3.16559200
C	-4.08531100	3.77170900	-2.21464800
H	-3.67665800	4.43753500	-1.43856000
H	-4.83189800	4.34585700	-2.78255000
H	-4.59982700	2.93453300	-1.72255700
C	-2.30181600	4.48436400	-3.81288900
H	-3.04515100	5.09894400	-4.34331800
H	-1.81500600	5.11577400	-3.05373100
H	-1.53878900	4.17883100	-4.54435700
C	-3.64455300	2.40070600	-4.24891100
H	-2.90906400	2.04587900	-4.98622900
H	-4.13372600	1.52828100	-3.79402700
H	-4.40418200	2.98537100	-4.79027900
H	-2.87493100	2.11890300	1.45344300
C	-3.23686400	1.44261100	4.12376300
C	-3.99746600	0.13606200	4.40939400
H	-3.35252400	-0.61160900	4.89538700
H	-4.84552900	0.33968700	5.08157600
H	-4.38873700	-0.29487500	3.47598000

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  C                -2.67746500    2.02633200    5.42738600
  H                -2.10800300    2.94901400    5.23649100
  H                -3.50608900    2.27220200    6.10857100
  H                -2.01844900    1.31915400    5.95205400
  C                -4.20593500    2.44710900    3.49926000
  H                -3.70431400    3.39516800    3.24987200
  H                -4.67444000    2.04770600    2.58840500
  H                -5.00783000    2.67300600    4.21725100
  P                -4.88222500   -0.23329700   -0.31956600
  F                -3.28196900   -0.50534700   -0.11459700
  F                -5.15951800   -0.75892500    1.19502900
  F                -4.69104100    1.29448300    0.26211700
  F                -6.46511700    0.05660000   -0.52110100
  F                -4.58137700    0.32513200   -1.82276900
  F                -5.06481200   -1.73368500   -0.89994200
-1 2
 Ir                1.40318200   -0.37401300   -0.05211600
 C                -0.83621300   -4.32254200   -1.66326200
 C                -1.42325800   -3.58895800   -0.60636400
 C                -0.80612500   -2.43002300   -0.17584200
 C                 0.92035700   -2.66529800   -1.77116200
 C                 0.32345900   -3.85285000   -2.23969600
 H                -1.29516200   -5.24572700   -2.02092400
 H                -1.23392000   -1.83910300    0.63346000
 H                 0.78848400   -4.39373200   -3.06024400
 C                 3.60478700   -0.06766700   -2.08876000
 C                 2.49998200   -0.80157100   -1.62365900
 C                 2.09553300   -2.01870600   -2.28646600
 C                 2.88512200   -2.45170800   -3.36931700
 C                 3.97132200   -1.73130600   -3.82551300
 C                 4.31557700   -0.53517100   -3.17555600
 H                 3.92221700    0.85650400   -1.60471600
 H                 4.54938600   -2.09222400   -4.67701800
 N                 0.33647300   -1.98930700   -0.71358300
 F                 2.59013300   -3.58864900   -4.00060800
 F                 5.36387400    0.14568600   -3.63227700
 C                -2.65984300   -4.09853100    0.06319600
 F                -3.09760200   -3.28073300    1.01799800
 F                -2.43208200   -5.29331600    0.63928700
 F                -3.65252900   -4.28943300   -0.81040100
 C                -2.09305600    1.09710400    3.18093000
 C                -1.03065800    0.28598200    3.60558600
 C                -0.04906400   -0.09586500    2.70892700
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C	-1.06482600	1.07420000	0.98787300
C	-2.07131500	1.50583000	1.84824400
H	-0.96391600	-0.07423600	4.63264300
H	0.77890800	-0.73891000	3.01303500
C	-1.94722100	2.44650300	-2.43791500
C	-2.00613600	2.19029700	-1.06827900
C	-1.03373000	1.41025300	-0.44771800
C	0.07077600	1.12269000	-2.46202800
C	-0.86524200	1.88877600	-3.13348900
H	-2.83948700	2.56203400	-0.48055200
H	0.92004800	0.67759100	-2.98352900
H	-0.74099100	2.03755400	-4.20675500
N	-0.07403100	0.27505400	1.42216300
N	-0.00767100	0.89009300	-1.14571000
C	4.45031300	-1.31357400	2.66957400
C	4.29794600	-2.65101300	2.98754500
C	3.23564000	-3.35948100	2.41608600
C	2.34641900	-2.76344800	1.53945900
C	2.50583200	-1.40710400	1.21804500
C	3.56864500	-0.63987300	1.80627300
H	4.99543700	-3.13663800	3.67069400
H	1.54307700	-3.36409700	1.11142800
C	4.38231700	3.05029600	1.56931200
C	4.52216200	1.72680500	1.93175000
C	3.61206300	0.76067000	1.46329800
C	2.45284900	2.43580100	0.27353800
C	3.31036600	3.41891700	0.72617100
H	5.08880400	3.79863900	1.93236400
H	5.33265300	1.41947100	2.58798600
H	1.62827400	2.67690200	-0.39811700
F	3.09398500	-4.64415900	2.73153600
F	5.47571900	-0.66385800	3.22175000
N	2.60023200	1.14954800	0.60903300
C	3.11514500	4.84666300	0.32801900
F	4.20379400	5.34239900	-0.27396600
F	2.88136800	5.62591200	1.39223500
F	2.08768500	4.99993100	-0.51200400
C	-2.99550000	3.27650600	-3.16559200
C	-4.08531100	3.77170900	-2.21464800
H	-3.67665800	4.43753500	-1.43856000
H	-4.83189800	4.34585700	-2.78255000
H	-4.59982700	2.93453300	-1.72255700
C	-2.30181600	4.48436400	-3.81288900

H	-3.04515100	5.09894400	-4.34331800
H	-1.81500600	5.11577400	-3.05373100
H	-1.53878900	4.17883100	-4.54435700
C	-3.64455300	2.40070600	-4.24891100
H	-2.90906400	2.04587900	-4.98622900
H	-4.13372600	1.52828100	-3.79402700
H	-4.40418200	2.98537100	-4.79027900
H	-2.87493100	2.11890300	1.45344300
C	-3.23686400	1.44261100	4.12376300
C	-3.99746600	0.13606200	4.40939400
H	-3.35252400	-0.61160900	4.89538700
H	-4.84552900	0.33968700	5.08157600
H	-4.38873700	-0.29487500	3.47598000
C	-2.67746500	2.02633200	5.42738600
H	-2.10800300	2.94901400	5.23649100
H	-3.50608900	2.27220200	6.10857100
H	-2.01844900	1.31915400	5.95205400
C	-4.20593500	2.44710900	3.49926000
H	-3.70431400	3.39516800	3.24987200
H	-4.67444000	2.04770600	2.58840500
H	-5.00783000	2.67300600	4.21725100
P	-4.88222500	-0.23329700	-0.31956600
F	-3.28196900	-0.50534700	-0.11459700
F	-5.15951800	-0.75892500	1.19502900
F	-4.69104100	1.29448300	0.26211700
F	-6.46511700	0.05660000	-0.52110100
F	-4.58137700	0.32513200	-1.82276900
F	-5.06481200	-1.73368500	-0.89994200

SET2

C2-B2

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Ir	2.40410200	-0.88976700	-0.08856300
C	4.74025300	3.29542700	-0.58453600
C	3.69581400	3.00239400	-1.45950800
C	3.01261400	1.81062100	-1.29859900
C	4.43772900	1.12652100	0.42662200
C	5.11023100	2.35473300	0.36055300
H	5.27278100	4.24573500	-0.65085700
H	2.16455700	1.56846600	-1.93581700
H	5.93912700	2.54900800	1.03514400
C	4.36052200	-2.36308500	1.73976000
C	4.01491300	-1.19369600	1.05473600

C	4.80151400	-0.02189200	1.24850000
C	5.87641000	-0.07161400	2.14794000
C	6.21316900	-1.22198300	2.84187000
C	5.44154700	-2.35545700	2.61171000
H	3.80351200	-3.29346300	1.62061100
H	7.05427200	-1.23173600	3.53447700
N	3.36479100	0.90471300	-0.38181100
F	6.62397300	1.01171600	2.36900600
F	5.75600900	-3.47434000	3.26076900
C	3.36372500	3.92794500	-2.59285300
F	2.27272400	3.53664100	-3.25595100
F	4.37187800	3.94847100	-3.48188000
F	3.18181900	5.18334500	-2.19640400
C	-1.09062700	1.67735000	-2.32860800
C	-0.41578700	0.69545900	-3.06974100
C	0.44083200	-0.19000200	-2.43112300
C	-0.09344100	0.68387200	-0.36086400
C	-0.94449000	1.61858300	-0.94374800
H	-0.50325800	0.64250000	-4.15604500
H	1.03180200	-0.91472900	-2.99517600
C	-0.40888800	1.27257500	3.35903100
C	-0.72895200	1.23743000	2.00333500
C	0.14025700	0.64610500	1.09120900
C	1.58489900	0.03626900	2.78803700
C	0.78495800	0.64403200	3.74021300
H	-1.64789100	1.68860100	1.63675100
H	2.51585300	-0.46443300	3.06320800
H	1.10912400	0.62467000	4.78156600
N	0.63907200	-0.16579900	-1.10789800
N	1.26961400	0.03314600	1.48806200
C	3.24938800	-3.89406600	-2.93460600
C	4.05885100	-3.33412600	-3.90715900
C	4.44755600	-2.00919900	-3.72950100
C	4.04781500	-1.24835700	-2.63943200
C	3.21765300	-1.81400000	-1.66586900
C	2.81925700	-3.17472000	-1.80915000
H	4.37792700	-3.91354400	-4.77305000
H	4.39513800	-0.21619700	-2.57270100
C	0.98453800	-5.42678600	0.62700300
C	1.63856600	-5.04726600	-0.53190600
C	2.01409900	-3.70760200	-0.72067600
C	1.02361900	-3.13952500	1.32614600
C	0.68197400	-4.45555100	1.58420400

H	0.71846500	-6.47364200	0.78770100
H	1.89697500	-5.78646400	-1.28516600
H	0.78219900	-2.34820600	2.03382000
F	5.23301100	-1.45735900	-4.65086500
F	2.87660400	-5.16479200	-3.10588300
N	1.67532200	-2.77795300	0.21696500
C	0.02049200	-4.83208200	2.87742700
F	0.81106200	-5.61425400	3.61718000
F	-1.11191000	-5.51641200	2.66752700
F	-0.28796900	-3.76137600	3.61212600
C	-1.28124500	1.97543500	4.38925000
C	-2.47641800	2.66388400	3.73375800
H	-3.12859800	1.95006200	3.21036400
H	-3.08010900	3.16853300	4.50249700
H	-2.15140400	3.41976500	3.00364900
C	-1.78589500	0.93742900	5.40154200
H	-2.41093500	1.42823600	6.16354400
H	-2.39523800	0.16715500	4.90335200
H	-0.95713500	0.43257700	5.92030700
C	-0.43026100	3.04118200	5.09752300
H	0.41501900	2.59785800	5.64444600
H	-0.02857500	3.76381600	4.37141700
H	-1.04941000	3.58659500	5.82641300
H	-1.42436700	2.35187300	-0.30321300
C	-1.89674800	2.77556400	-3.01147200
C	-0.94445300	3.56868900	-3.91981900
H	-0.48186300	2.93106900	-4.68791000
H	-1.50162800	4.36667900	-4.43438900
H	-0.14262400	4.02823300	-3.32530400
C	-3.01395200	2.14270300	-3.85109600
H	-3.71827400	1.57541800	-3.22370500
H	-3.58669400	2.92798800	-4.36744800
H	-2.61819800	1.46062800	-4.61834400
C	-2.50490400	3.74624900	-1.99708800
H	-3.19246200	3.24644400	-1.29914800
H	-1.72514700	4.24662300	-1.40489900
H	-3.07726900	4.51971900	-2.52974400
P	0.99499500	4.55099300	0.82270600
F	0.90953800	4.07321200	-0.73932800
F	0.36210100	5.98948100	0.41487700
F	-0.51893500	3.96991400	1.06688600
F	1.05867700	5.00453300	2.38507900
F	1.62452800	3.09801700	1.22033000

F	2.49282200	5.12991200	0.58181000
C	-5.65002400	1.77310300	0.92380800
C	-5.74251900	2.88934900	1.95718200
H	-5.40529500	2.54993100	2.94641700
H	-5.10245900	3.72848400	1.64737100
H	-6.77231300	3.25963100	2.04814800
C	-6.18712000	2.26338600	-0.43499200
H	-5.53629800	3.05820700	-0.83076400
H	-6.23511100	1.43819700	-1.16192400
H	-7.19016800	2.68964400	-0.31358200
C	-7.73815200	0.30927100	1.89450500
N	-4.22650500	1.50346800	0.70782900
C	-3.79349800	0.57752000	-0.19080200
C	-3.23623200	-0.69137100	0.09215100
C	-3.18328600	-1.25324200	1.39663200
C	-2.71229200	-1.46267100	-0.98091000
C	-2.71654500	-2.54491400	1.58853900
C	-2.24145100	-2.74704000	-0.77444500
C	-2.26394500	-3.31180000	0.50688500
H	-2.70458500	-2.96814200	2.59579300
H	-1.86190900	-3.32674600	-1.62011100
C	-6.29072400	0.43466200	1.36463100
H	-5.64059800	0.00897200	2.14659600
H	-6.19426500	-0.23450400	0.49505500
C	-8.02612600	-1.19823200	1.93776700
H	-9.02147000	-1.39345900	2.36680700
H	-8.00264400	-1.63954400	0.92883600
H	-7.28139500	-1.72845000	2.55273500
C	-7.88459400	0.84967900	3.32110100
H	-7.13409800	0.40220700	3.99225200
H	-7.77681600	1.94072500	3.37333800
H	-8.88082700	0.59895000	3.71896800
C	-8.77744700	0.96990100	0.98703400
H	-8.70887600	2.06733500	1.01045700
H	-8.66858400	0.64197200	-0.05842300
H	-9.79231300	0.70047600	1.32029800
H	-3.76776800	0.92019600	-1.23232700
N	-5.53521900	-2.99925600	-2.22963800
C	-5.83055100	-1.76787100	-2.78844700
N	-5.32628500	-1.57084700	-4.06134300
N	-6.51939600	-0.83562400	-2.21943600
H	-6.98051900	-1.19795800	-1.38636600
C	-5.73283100	-3.18384800	-0.81691900

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 H                -6.78622400   -3.40848400   -0.55299200
 C                -5.58092700   -4.21174900   -3.01479600
 H                -5.65698900   -3.96948600   -4.08087900
 H                -4.68070800   -4.82975200   -2.85512600
 H                -6.46228200   -4.82167300   -2.74229100
 C                -3.98189600   -1.97147000   -4.40517600
 H                -3.94844500   -2.44170300   -5.40225500
 H                -3.29974900   -1.09977900   -4.42267700
 H                -3.59572800   -2.68500000   -3.66915000
 C                -5.84557200   -0.47211600   -4.83395300
 H                -5.70566300   -0.68499300   -5.90551000
 H                -6.91419300   -0.34445400   -4.62496300
 H                -5.34266700    0.48630500   -4.60630700
 H                -2.70938400   -1.03107400   -1.98371000
 H                -3.52515900   -0.66423900    2.25025300
 H                -1.93128200   -4.33799200    0.66256100

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 Ir                2.40410200   -0.88976700   -0.08856300
 C                 4.74025300    3.29542700   -0.58453600
 C                 3.69581400    3.00239400   -1.45950800
 C                 3.01261400    1.81062100   -1.29859900
 C                 4.43772900    1.12652100    0.42662200
 C                 5.11023100    2.35473300    0.36055300
 H                 5.27278100    4.24573500   -0.65085700
 H                 2.16455700    1.56846600   -1.93581700
 H                 5.93912700    2.54900800    1.03514400
 C                 4.36052200   -2.36308500    1.73976000
 C                 4.01491300   -1.19369600    1.05473600
 C                 4.80151400   -0.02189200    1.24850000
 C                 5.87641000   -0.07161400    2.14794000
 C                 6.21316900   -1.22198300    2.84187000
 C                 5.44154700   -2.35545700    2.61171000
 H                 3.80351200   -3.29346300    1.62061100
 H                 7.05427200   -1.23173600    3.53447700
 N                 3.36479100    0.90471300   -0.38181100
 F                 6.62397300    1.01171600    2.36900600
 F                 5.75600900   -3.47434000    3.26076900
 C                 3.36372500    3.92794500   -2.59285300
 F                 2.27272400    3.53664100   -3.25595100
 F                 4.37187800    3.94847100   -3.48188000
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F	3.18181900	5.18334500	-2.19640400
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C	0.44083200	-0.19000200	-2.43112300
C	-0.09344100	0.68387200	-0.36086400
C	-0.94449000	1.61858300	-0.94374800
H	-0.50325800	0.64250000	-4.15604500
H	1.03180200	-0.91472900	-2.99517600
C	-0.40888800	1.27257500	3.35903100
C	-0.72895200	1.23743000	2.00333500
C	0.14025700	0.64610500	1.09120900
C	1.58489900	0.03626900	2.78803700
C	0.78495800	0.64403200	3.74021300
H	-1.64789100	1.68860100	1.63675100
H	2.51585300	-0.46443300	3.06320800
H	1.10912400	0.62467000	4.78156600
N	0.63907200	-0.16579900	-1.10789800
N	1.26961400	0.03314600	1.48806200
C	3.24938800	-3.89406600	-2.93460600
C	4.05885100	-3.33412600	-3.90715900
C	4.44755600	-2.00919900	-3.72950100
C	4.04781500	-1.24835700	-2.63943200
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C	2.81925700	-3.17472000	-1.80915000
H	4.37792700	-3.91354400	-4.77305000
H	4.39513800	-0.21619700	-2.57270100
C	0.98453800	-5.42678600	0.62700300
C	1.63856600	-5.04726600	-0.53190600
C	2.01409900	-3.70760200	-0.72067600
C	1.02361900	-3.13952500	1.32614600
C	0.68197400	-4.45555100	1.58420400
H	0.71846500	-6.47364200	0.78770100
H	1.89697500	-5.78646400	-1.28516600
H	0.78219900	-2.34820600	2.03382000
F	5.23301100	-1.45735900	-4.65086500
F	2.87660400	-5.16479200	-3.10588300
N	1.67532200	-2.77795300	0.21696500
C	0.02049200	-4.83208200	2.87742700
F	0.81106200	-5.61425400	3.61718000
F	-1.11191000	-5.51641200	2.66752700
F	-0.28796900	-3.76137600	3.61212600
C	-1.28124500	1.97543500	4.38925000
C	-2.47641800	2.66388400	3.73375800

H	-3.12859800	1.95006200	3.21036400
H	-3.08010900	3.16853300	4.50249700
H	-2.15140400	3.41976500	3.00364900
C	-1.78589500	0.93742900	5.40154200
H	-2.41093500	1.42823600	6.16354400
H	-2.39523800	0.16715500	4.90335200
H	-0.95713500	0.43257700	5.92030700
C	-0.43026100	3.04118200	5.09752300
H	0.41501900	2.59785800	5.64444600
H	-0.02857500	3.76381600	4.37141700
H	-1.04941000	3.58659500	5.82641300
H	-1.42436700	2.35187300	-0.30321300
C	-1.89674800	2.77556400	-3.01147200
C	-0.94445300	3.56868900	-3.91981900
H	-0.48186300	2.93106900	-4.68791000
H	-1.50162800	4.36667900	-4.43438900
H	-0.14262400	4.02823300	-3.32530400
C	-3.01395200	2.14270300	-3.85109600
H	-3.71827400	1.57541800	-3.22370500
H	-3.58669400	2.92798800	-4.36744800
H	-2.61819800	1.46062800	-4.61834400
C	-2.50490400	3.74624900	-1.99708800
H	-3.19246200	3.24644400	-1.29914800
H	-1.72514700	4.24662300	-1.40489900
H	-3.07726900	4.51971900	-2.52974400
P	0.99499500	4.55099300	0.82270600
F	0.90953800	4.07321200	-0.73932800
F	0.36210100	5.98948100	0.41487700
F	-0.51893500	3.96991400	1.06688600
F	1.05867700	5.00453300	2.38507900
F	1.62452800	3.09801700	1.22033000
F	2.49282200	5.12991200	0.58181000
C	-5.65002400	1.77310300	0.92380800
C	-5.74251900	2.88934900	1.95718200
H	-5.40529500	2.54993100	2.94641700
H	-5.10245900	3.72848400	1.64737100
H	-6.77231300	3.25963100	2.04814800
C	-6.18712000	2.26338600	-0.43499200
H	-5.53629800	3.05820700	-0.83076400
H	-6.23511100	1.43819700	-1.16192400
H	-7.19016800	2.68964400	-0.31358200
C	-7.73815200	0.30927100	1.89450500
N	-4.22650500	1.50346800	0.70782900

C	-3.79349800	0.57752000	-0.19080200
C	-3.23623200	-0.69137100	0.09215100
C	-3.18328600	-1.25324200	1.39663200
C	-2.71229200	-1.46267100	-0.98091000
C	-2.71654500	-2.54491400	1.58853900
C	-2.24145100	-2.74704000	-0.77444500
C	-2.26394500	-3.31180000	0.50688500
H	-2.70458500	-2.96814200	2.59579300
H	-1.86190900	-3.32674600	-1.62011100
C	-6.29072400	0.43466200	1.36463100
H	-5.64059800	0.00897200	2.14659600
H	-6.19426500	-0.23450400	0.49505500
C	-8.02612600	-1.19823200	1.93776700
H	-9.02147000	-1.39345900	2.36680700
H	-8.00264400	-1.63954400	0.92883600
H	-7.28139500	-1.72845000	2.55273500
C	-7.88459400	0.84967900	3.32110100
H	-7.13409800	0.40220700	3.99225200
H	-7.77681600	1.94072500	3.37333800
H	-8.88082700	0.59895000	3.71896800
C	-8.77744700	0.96990100	0.98703400
H	-8.70887600	2.06733500	1.01045700
H	-8.66858400	0.64197200	-0.05842300
H	-9.79231300	0.70047600	1.32029800
H	-3.76776800	0.92019600	-1.23232700
N	-5.53521900	-2.99925600	-2.22963800
C	-5.83055100	-1.76787100	-2.78844700
N	-5.32628500	-1.57084700	-4.06134300
N	-6.51939600	-0.83562400	-2.21943600
H	-6.98051900	-1.19795800	-1.38636600
C	-5.73283100	-3.18384800	-0.81691900
H	-5.11288300	-4.02428300	-0.47210900
H	-5.40836900	-2.29140000	-0.26541800
H	-6.78622400	-3.40848400	-0.55299200
C	-5.58092700	-4.21174900	-3.01479600
H	-5.65698900	-3.96948600	-4.08087900
H	-4.68070800	-4.82975200	-2.85512600
H	-6.46228200	-4.82167300	-2.74229100
C	-3.98189600	-1.97147000	-4.40517600
H	-3.94844500	-2.44170300	-5.40225500
H	-3.29974900	-1.09977900	-4.42267700
H	-3.59572800	-2.68500000	-3.66915000
C	-5.84557200	-0.47211600	-4.83395300

H	-5.70566300	-0.68499300	-5.90551000
H	-6.91419300	-0.34445400	-4.62496300
H	-5.34266700	0.48630500	-4.60630700
H	-2.70938400	-1.03107400	-1.98371000
H	-3.52515900	-0.66423900	2.25025300
H	-1.93128200	-4.33799200	0.66256100

SET3

M5-M7

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C	-2.13108500	0.75354700	-1.27070300
H	-1.18295000	1.31106200	-1.28494500
H	-2.54006900	0.75704900	-2.29244700
H	-2.82427100	1.29929400	-0.61660000
C	-0.79804100	-1.29661500	-1.68116600
H	0.13947000	-0.72484100	-1.63391600
H	-0.58203300	-2.33547800	-1.38320200
H	-1.12539900	-1.31002600	-2.73262900
C	-1.38604100	-0.68641400	0.68670900
H	-2.21503800	-0.42361800	1.34837800
H	-1.08710700	-1.71553700	0.93695700
C	-0.27018500	0.24504100	0.99252400
C	-0.46782200	1.52690200	1.65865700
O	0.43447400	2.25054100	2.03785100
O	-1.76193100	1.82888200	1.82133100
C	-2.04032600	3.06068400	2.46418500
H	-1.64898900	3.90380200	1.87580700
H	-3.13136000	3.12805200	2.53814000
H	-1.58939900	3.09089700	3.46646500
N	1.04827900	-0.05622300	0.64743100
C	1.91904700	0.94496400	0.12955600
C	1.54139800	-1.36250100	0.84859800
O	3.09434600	0.98243400	0.37210300
O	1.10078800	-2.09576700	1.69804200
O	1.23462700	1.74990700	-0.66031600
O	2.46438900	-1.63925500	-0.04704800
C	1.82605200	2.96088000	-1.23289000
C	3.29378400	-2.84099000	0.03271400
C	2.42500900	-4.07092700	-0.18475600
H	3.06470000	-4.96304800	-0.25065300
H	1.71497200	-4.20614200	0.64044900
H	1.86475900	-3.97942400	-1.12729700
C	4.02277100	-2.86641400	1.36781000

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 H                3.32525900   -3.00644100    2.20335900
 H                4.74411600   -3.69606900    1.37237400
 H                4.57469500   -1.92658200    1.51613800
 C                4.26921700   -2.64950900   -1.11644000
 H                4.96337500   -3.49999100   -1.16543900
 H                3.72973300   -2.58163400   -2.07233100
 H                4.84998400   -1.72654100   -0.97648000
 C                2.38059200    3.85042300   -0.12986900
 H                3.26229100    3.40163200    0.34369400
 H                2.66946500    4.81855600   -0.56393200
 H                1.61622800    4.01973700    0.64097500
 C                2.88597100    2.55727800   -2.24673700
 H                3.27301400    3.45544700   -2.74953700
 H                3.72218500    2.04132600   -1.75807100
 H                2.45321600    1.89458600   -3.01099400
 C                0.64086100    3.62447000   -1.91424600
 H                0.96441200    4.55184000   -2.40731500
 H                0.20618600    2.95854600   -2.67360100
 H               -0.13727700    3.87240800   -1.17768300
 C               -1.88414700   -0.67717200   -0.79224300
 C               -3.12202900   -1.59923700   -0.90300000
 H               -3.20857900   -1.89207300   -1.96430300
 H               -2.85886600   -2.53035900   -0.36978900
 C               -4.55286100   -1.20117600   -0.45983400
 C               -5.37654100   -2.49631000   -0.49322400
 H               -6.42912900   -2.29828200   -0.23533300
 H               -5.35535000   -2.95456700   -1.49520100
 H               -4.98508400   -3.23563400    0.22363500
 C               -4.63229400   -0.62440200    0.95602900
 H               -4.20634300   -1.31642200    1.69961100
 H               -4.10890600    0.33903400    1.04543100
 H               -5.68570000   -0.45313500    1.23063600
 C               -5.20328300   -0.21681500   -1.43972800
 H               -4.74001800    0.77737300   -1.40775700
 H               -5.13720500   -0.58815400   -2.47498000
 H               -6.27077100   -0.09126800   -1.19702300
-1 1
 C               -2.13108500    0.75354700   -1.27070300
 H               -1.18295000    1.31106200   -1.28494500
 H               -2.54006900    0.75704900   -2.29244700
 H               -2.82427100    1.29929400   -0.61660000
 C               -0.79804100   -1.29661500   -1.68116600
 H                0.13947000   -0.72484100   -1.63391600
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H	-0.58203300	-2.33547800	-1.38320200
H	-1.12539900	-1.31002600	-2.73262900
C	-1.38604100	-0.68641400	0.68670900
H	-2.21503800	-0.42361800	1.34837800
H	-1.08710700	-1.71553700	0.93695700
C	-0.27018500	0.24504100	0.99252400
C	-0.46782200	1.52690200	1.65865700
O	0.43447400	2.25054100	2.03785100
O	-1.76193100	1.82888200	1.82133100
C	-2.04032600	3.06068400	2.46418500
H	-1.64898900	3.90380200	1.87580700
H	-3.13136000	3.12805200	2.53814000
H	-1.58939900	3.09089700	3.46646500
N	1.04827900	-0.05622300	0.64743100
C	1.91904700	0.94496400	0.12955600
C	1.54139800	-1.36250100	0.84859800
O	3.09434600	0.98243400	0.37210300
O	1.10078800	-2.09576700	1.69804200
O	1.23462700	1.74990700	-0.66031600
O	2.46438900	-1.63925500	-0.04704800
C	1.82605200	2.96088000	-1.23289000
C	3.29378400	-2.84099000	0.03271400
C	2.42500900	-4.07092700	-0.18475600
H	3.06470000	-4.96304800	-0.25065300
H	1.71497200	-4.20614200	0.64044900
H	1.86475900	-3.97942400	-1.12729700
C	4.02277100	-2.86641400	1.36781000
H	3.32525900	-3.00644100	2.20335900
H	4.74411600	-3.69606900	1.37237400
H	4.57469500	-1.92658200	1.51613800
C	4.26921700	-2.64950900	-1.11644000
H	4.96337500	-3.49999100	-1.16543900
H	3.72973300	-2.58163400	-2.07233100
H	4.84998400	-1.72654100	-0.97648000
C	2.38059200	3.85042300	-0.12986900
H	3.26229100	3.40163200	0.34369400
H	2.66946500	4.81855600	-0.56393200
H	1.61622800	4.01973700	0.64097500
C	2.88597100	2.55727800	-2.24673700
H	3.27301400	3.45544700	-2.74953700
H	3.72218500	2.04132600	-1.75807100
H	2.45321600	1.89458600	-3.01099400
C	0.64086100	3.62447000	-1.91424600

H	0.96441200	4.55184000	-2.40731500
H	0.20618600	2.95854600	-2.67360100
H	-0.13727700	3.87240800	-1.17768300
C	-1.88414700	-0.67717200	-0.79224300
C	-3.12202900	-1.59923700	-0.90300000
H	-3.20857900	-1.89207300	-1.96430300
H	-2.85886600	-2.53035900	-0.36978900
C	-4.55286100	-1.20117600	-0.45983400
C	-5.37654100	-2.49631000	-0.49322400
H	-6.42912900	-2.29828200	-0.23533300
H	-5.35535000	-2.95456700	-1.49520100
H	-4.98508400	-3.23563400	0.22363500
C	-4.63229400	-0.62440200	0.95602900
H	-4.20634300	-1.31642200	1.69961100
H	-4.10890600	0.33903400	1.04543100
H	-5.68570000	-0.45313500	1.23063600
C	-5.20328300	-0.21681500	-1.43972800
H	-4.74001800	0.77737300	-1.40775700
H	-5.13720500	-0.58815400	-2.47498000
H	-6.27077100	-0.09126800	-1.19702300

Ir(II)-Ir(III)

-1 2

Ir	1.43810800	-0.36770400	-0.08642700
C	-1.41285800	-3.52711200	-2.31850500
C	-1.74824300	-3.09391200	-1.03444500
C	-0.92751900	-2.16840300	-0.41166500
C	0.55199000	-2.12696900	-2.23299800
C	-0.26551900	-3.03787600	-2.91919600
H	-2.04563600	-4.24351600	-2.84603400
H	-1.16125900	-1.77494500	0.57682500
H	0.01357400	-3.36197000	-3.91789200
C	3.69920100	-0.12925600	-2.14376500
C	2.46920700	-0.69020400	-1.77778300
C	1.81332700	-1.56124700	-2.69642500
C	2.41378900	-1.81398700	-3.93839900
C	3.62507000	-1.25329800	-4.30708400
C	4.24666300	-0.41483900	-3.38612100
H	4.24584400	0.53937000	-1.47562000
H	4.06788000	-1.46552400	-5.27977700
N	0.18750600	-1.70895900	-0.98812000
F	1.82236400	-2.61973300	-4.82708100
F	5.41579000	0.13107700	-3.72391700

C	-2.92694900	-3.67438600	-0.31030700
F	-3.29025500	-2.94160000	0.73741400
F	-2.63522000	-4.90386200	0.15333600
F	-3.97983200	-3.81437800	-1.11548900
C	-2.06933500	0.32484100	3.29655700
C	-0.94528600	-0.49946400	3.61499800
C	0.07399500	-0.62981900	2.69813600
C	-0.94723300	0.85657400	1.19171200
C	-2.03787200	0.99340200	2.09410200
H	-0.88693200	-1.05267300	4.55268100
H	0.92649200	-1.28609800	2.89484200
C	-1.69124900	3.05616700	-1.77594000
C	-1.81023500	2.46549500	-0.53847300
C	-0.86511500	1.51302000	-0.07020800
C	0.32173300	1.74891000	-2.08214300
C	-0.56796300	2.67880000	-2.57274700
H	-2.65905400	2.69788600	0.09885300
H	1.18589700	1.43257100	-2.67269500
H	-0.40272100	3.09567500	-3.56656600
N	0.08755000	-0.00110300	1.51265000
N	0.20142800	1.17351500	-0.87617400
C	4.49689200	-2.01871300	2.32749300
C	4.32536700	-3.39181000	2.34359000
C	3.26725100	-3.91164500	1.60164500
C	2.40218600	-3.11426400	0.86737800
C	2.57469800	-1.72430000	0.85659200
C	3.65239400	-1.16343400	1.60382100
H	4.99430800	-4.03419500	2.91551800
H	1.59540700	-3.59531200	0.31079100
C	4.70774200	2.46056800	2.00690800
C	4.73627200	1.08671700	2.16435500
C	3.76470000	0.28666000	1.54065000
C	2.76668700	2.20547800	0.62945300
C	3.70034200	3.03558500	1.22619700
H	5.46475300	3.08319900	2.48822700
H	5.50834500	0.61788600	2.76828300
H	1.96019500	2.59765600	0.00923600
F	3.09025000	-5.23294000	1.60604300
F	5.51321600	-1.52310500	3.04204500
N	2.80158800	0.87709300	0.77749000
C	3.62996900	4.52270700	1.04719700
F	4.77725900	5.00786700	0.55779300
F	3.41555400	5.14573900	2.21180500

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 F                 2.65240600    4.88183000    0.21424500
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 H                -3.35106400    4.87368900   -0.41016600
 H                -4.50929600    5.09753700   -1.74103100
 H                -4.34223900    3.50145100   -0.96961800
 C                -2.00987500    5.33077900   -2.76558100
 H                -2.74329000    6.04551200   -3.17169700
 H                -1.50407500    5.80925500   -1.91212900
 H                -1.25635300    5.14726700   -3.54579400
 C                -3.40030100    3.38474500   -3.54037500
 H                -2.67201200    3.12214900   -4.32261600
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 H                -4.13695400    4.07534500   -3.98218000
 H                -2.88644200    1.59631100    1.78048900
 C                -3.26033900    0.38110000    4.24605200
 C                -3.90040200   -1.01635500    4.28817900
 H                -3.18507700   -1.77839800    4.63336400
 H                -4.76122000   -1.02314300    4.97645900
 H                -4.25416600   -1.30275000    3.28676700
 C                -2.78365000    0.77714600    5.65016100
 H                -2.31567300    1.77413800    5.63937700
 H                -3.63744500    0.80893500    6.34564800
 H                -2.05083200    0.06380000    6.05548900
 C                -4.31681100    1.38512000    3.78408100
 H                -3.90486500    2.40479600    3.72473300
 H                -4.72363600    1.11770700    2.79933200
 H                -5.15017300    1.40168200    4.50351600
 P                -5.14760500    0.05905400   -0.45263200
 F                -3.56331700   -0.28892000   -0.58206000
 F                -5.19678400   -0.66229900    1.00827300
 F                -4.78289700    1.48394500    0.27487700
 F                -6.73015500    0.41778800   -0.32437200
 F                -5.10290900    0.80004000   -1.90659800
 F                -5.52205300   -1.34762500   -1.17360700
0 1
 Ir                1.43810800   -0.36770400   -0.08642700
 C                -1.41285800   -3.52711200   -2.31850500
 C                -1.74824300   -3.09391200   -1.03444500
 C                -0.92751900   -2.16840300   -0.41166500
 C                 0.55199000   -2.12696900   -2.23299800
 C                -0.26551900   -3.03787600   -2.91919600
 H                -2.04563600   -4.24351600   -2.84603400
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H	-1.16125900	-1.77494500	0.57682500
H	0.01357400	-3.36197000	-3.91789200
C	3.69920100	-0.12925600	-2.14376500
C	2.46920700	-0.69020400	-1.77778300
C	1.81332700	-1.56124700	-2.69642500
C	2.41378900	-1.81398700	-3.93839900
C	3.62507000	-1.25329800	-4.30708400
C	4.24666300	-0.41483900	-3.38612100
H	4.24584400	0.53937000	-1.47562000
H	4.06788000	-1.46552400	-5.27977700
N	0.18750600	-1.70895900	-0.98812000
F	1.82236400	-2.61973300	-4.82708100
F	5.41579000	0.13107700	-3.72391700
C	-2.92694900	-3.67438600	-0.31030700
F	-3.29025500	-2.94160000	0.73741400
F	-2.63522000	-4.90386200	0.15333600
F	-3.97983200	-3.81437800	-1.11548900
C	-2.06933500	0.32484100	3.29655700
C	-0.94528600	-0.49946400	3.61499800
C	0.07399500	-0.62981900	2.69813600
C	-0.94723300	0.85657400	1.19171200
C	-2.03787200	0.99340200	2.09410200
H	-0.88693200	-1.05267300	4.55268100
H	0.92649200	-1.28609800	2.89484200
C	-1.69124900	3.05616700	-1.77594000
C	-1.81023500	2.46549500	-0.53847300
C	-0.86511500	1.51302000	-0.07020800
C	0.32173300	1.74891000	-2.08214300
C	-0.56796300	2.67880000	-2.57274700
H	-2.65905400	2.69788600	0.09885300
H	1.18589700	1.43257100	-2.67269500
H	-0.40272100	3.09567500	-3.56656600
N	0.08755000	-0.00110300	1.51265000
N	0.20142800	1.17351500	-0.87617400
C	4.49689200	-2.01871300	2.32749300
C	4.32536700	-3.39181000	2.34359000
C	3.26725100	-3.91164500	1.60164500
C	2.40218600	-3.11426400	0.86737800
C	2.57469800	-1.72430000	0.85659200
C	3.65239400	-1.16343400	1.60382100
H	4.99430800	-4.03419500	2.91551800
H	1.59540700	-3.59531200	0.31079100
C	4.70774200	2.46056800	2.00690800

C	4.73627200	1.08671700	2.16435500
C	3.76470000	0.28666000	1.54065000
C	2.76668700	2.20547800	0.62945300
C	3.70034200	3.03558500	1.22619700
H	5.46475300	3.08319900	2.48822700
H	5.50834500	0.61788600	2.76828300
H	1.96019500	2.59765600	0.00923600
F	3.09025000	-5.23294000	1.60604300
F	5.51321600	-1.52310500	3.04204500
N	2.80158800	0.87709300	0.77749000
C	3.62996900	4.52270700	1.04719700
F	4.77725900	5.00786700	0.55779300
F	3.41555400	5.14573900	2.21180500
F	2.65240600	4.88183000	0.21424500
C	-2.71630800	4.03969100	-2.32942400
C	-3.78907500	4.39212000	-1.29859100
H	-3.35106400	4.87368900	-0.41016600
H	-4.50929600	5.09753700	-1.74103100
H	-4.34223900	3.50145100	-0.96961800
C	-2.00987500	5.33077900	-2.76558100
H	-2.74329000	6.04551200	-3.17169700
H	-1.50407500	5.80925500	-1.91212900
H	-1.25635300	5.14726700	-3.54579400
C	-3.40030100	3.38474500	-3.54037500
H	-2.67201200	3.12214900	-4.32261600
H	-3.92380200	2.46792100	-3.23201200
H	-4.13695400	4.07534500	-3.98218000
H	-2.88644200	1.59631100	1.78048900
C	-3.26033900	0.38110000	4.24605200
C	-3.90040200	-1.01635500	4.28817900
H	-3.18507700	-1.77839800	4.63336400
H	-4.76122000	-1.02314300	4.97645900
H	-4.25416600	-1.30275000	3.28676700
C	-2.78365000	0.77714600	5.65016100
H	-2.31567300	1.77413800	5.63937700
H	-3.63744500	0.80893500	6.34564800
H	-2.05083200	0.06380000	6.05548900
C	-4.31681100	1.38512000	3.78408100
H	-3.90486500	2.40479600	3.72473300
H	-4.72363600	1.11770700	2.79933200
H	-5.15017300	1.40168200	4.50351600
P	-5.14760500	0.05905400	-0.45263200
F	-3.56331700	-0.28892000	-0.58206000

F	-5.19678400	-0.66229900	1.00827300
F	-4.78289700	1.48394500	0.27487700
F	-6.73015500	0.41778800	-0.32437200
F	-5.10290900	0.80004000	-1.90659800
F	-5.52205300	-1.34762500	-1.17360700

SET4

Ra-^{2}Sa

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C	-1.09679900	0.66761300	0.47986200
C	-1.51081700	0.67709900	1.95380400
H	-1.45717500	-0.33318600	2.38332100
H	-0.82592400	1.32567300	2.52150500
H	-2.52959300	1.06708500	2.08471200
C	-1.22590200	2.07974900	-0.09155700
H	-0.56491900	2.77977900	0.44356900
H	-0.97157700	2.11544000	-1.16196400
H	-2.25129100	2.45146500	0.01569800
C	-3.39722500	-0.54551500	-0.38593400
N	0.27444900	0.14999500	0.48074200
C	1.23256200	0.75456200	-0.08884000
H	1.11239300	1.71743500	-0.61761800
C	2.60467500	0.21634400	-0.09578500
C	2.91378000	-0.99840600	0.53432500
C	3.62237000	0.92675200	-0.74444600
C	4.21403800	-1.48890500	0.51311800
C	4.92676800	0.43479400	-0.76592600
C	5.22449900	-0.77369500	-0.13737200
H	4.44744000	-2.43603600	1.00583800
H	5.71347800	0.99640200	-1.27525300
C	-1.85913000	-0.37813000	-0.37566100
H	-1.43573700	-1.35889900	-0.10220800
H	-1.53363500	-0.19959400	-1.41559600
C	-3.70229000	-1.47374500	-1.57028000
H	-4.77915200	-1.69956400	-1.62334600
H	-3.40505600	-1.01142800	-2.52499400
H	-3.16104600	-2.42879100	-1.47546300
C	-3.90972000	-1.23389100	0.88455600
H	-3.36397300	-2.17231500	1.07240500
H	-3.81074700	-0.60274300	1.77708500
H	-4.97747200	-1.48338600	0.77563000
C	-4.16205000	0.76227800	-0.59796700
H	-4.08341100	1.43461600	0.26913400

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 H                -3.79997500    1.30352500   -1.48594900
 H                -5.23282900    0.55069100   -0.74852400
 H                 2.10894100   -1.54021400    1.03548600
 H                 6.24599100   -1.16156200   -0.15281000
 H                 3.38556600    1.87422500   -1.23725100
1 2
 C                -1.09679900    0.66761300    0.47986200
 C                -1.51081700    0.67709900    1.95380400
 H                -1.45717500   -0.33318600    2.38332100
 H                -0.82592400    1.32567300    2.52150500
 H                -2.52959300    1.06708500    2.08471200
 C                -1.22590200    2.07974900   -0.09155700
 H                -0.56491900    2.77977900    0.44356900
 H                -0.97157700    2.11544000   -1.16196400
 H                -2.25129100    2.45146500    0.01569800
 C                -3.39722500   -0.54551500   -0.38593400
 N                 0.27444900    0.14999500    0.48074200
 C                 1.23256200    0.75456200   -0.08884000
 H                 1.11239300    1.71743500   -0.61761800
 C                 2.60467500    0.21634400   -0.09578500
 C                 2.91378000   -0.99840600    0.53432500
 C                 3.62237000    0.92675200   -0.74444600
 C                 4.21403800   -1.48890500    0.51311800
 C                 4.92676800    0.43479400   -0.76592600
 C                 5.22449900   -0.77369500   -0.13737200
 H                 4.44744000   -2.43603600    1.00583800
 H                 5.71347800    0.99640200   -1.27525300
 C                -1.85913000   -0.37813000   -0.37566100
 H                -1.43573700   -1.35889900   -0.10220800
 H                -1.53363500   -0.19959400   -1.41559600
 C                -3.70229000   -1.47374500   -1.57028000
 H                -4.77915200   -1.69956400   -1.62334600
 H                -3.40505600   -1.01142800   -2.52499400
 H                -3.16104600   -2.42879100   -1.47546300
 C                -3.90972000   -1.23389100    0.88455600
 H                -3.36397300   -2.17231500    1.07240500
 H                -3.81074700   -0.60274300    1.77708500
 H                -4.97747200   -1.48338600    0.77563000
 C                -4.16205000    0.76227800   -0.59796700
 H                -4.08341100    1.43461600    0.26913400
 H                -3.79997500    1.30352500   -1.48594900
 H                -5.23282900    0.55069100   -0.74852400
 H                 2.10894100   -1.54021400    1.03548600
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H	6.24599100	-1.16156200	-0.15281000
H	3.38556600	1.87422500	-1.23725100

Ir(III)*-Ir(II)

0 3

Ir	1.40318200	-0.37401300	-0.05211600
C	-0.83621300	-4.32254200	-1.66326200
C	-1.42325800	-3.58895800	-0.60636400
C	-0.80612500	-2.43002300	-0.17584200
C	0.92035700	-2.66529800	-1.77116200
C	0.32345900	-3.85285000	-2.23969600
H	-1.29516200	-5.24572700	-2.02092400
H	-1.23392000	-1.83910300	0.63346000
H	0.78848400	-4.39373200	-3.06024400
C	3.60478700	-0.06766700	-2.08876000
C	2.49998200	-0.80157100	-1.62365900
C	2.09553300	-2.01870600	-2.28646600
C	2.88512200	-2.45170800	-3.36931700
C	3.97132200	-1.73130600	-3.82551300
C	4.31557700	-0.53517100	-3.17555600
H	3.92221700	0.85650400	-1.60471600
H	4.54938600	-2.09222400	-4.67701800
N	0.33647300	-1.98930700	-0.71358300
F	2.59013300	-3.58864900	-4.00060800
F	5.36387400	0.14568600	-3.63227700
C	-2.65984300	-4.09853100	0.06319600
F	-3.09760200	-3.28073300	1.01799800
F	-2.43208200	-5.29331600	0.63928700
F	-3.65252900	-4.28943300	-0.81040100
C	-2.09305600	1.09710400	3.18093000
C	-1.03065800	0.28598200	3.60558600
C	-0.04906400	-0.09586500	2.70892700
C	-1.06482600	1.07420000	0.98787300
C	-2.07131500	1.50583000	1.84824400
H	-0.96391600	-0.07423600	4.63264300
H	0.77890800	-0.73891000	3.01303500
C	-1.94722100	2.44650300	-2.43791500
C	-2.00613600	2.19029700	-1.06827900
C	-1.03373000	1.41025300	-0.44771800
C	0.07077600	1.12269000	-2.46202800
C	-0.86524200	1.88877600	-3.13348900
H	-2.83948700	2.56203400	-0.48055200
H	0.92004800	0.67759100	-2.98352900

H	-0.74099100	2.03755400	-4.20675500
N	-0.07403100	0.27505400	1.42216300
N	-0.00767100	0.89009300	-1.14571000
C	4.45031300	-1.31357400	2.66957400
C	4.29794600	-2.65101300	2.98754500
C	3.23564000	-3.35948100	2.41608600
C	2.34641900	-2.76344800	1.53945900
C	2.50583200	-1.40710400	1.21804500
C	3.56864500	-0.63987300	1.80627300
H	4.99543700	-3.13663800	3.67069400
H	1.54307700	-3.36409700	1.11142800
C	4.38231700	3.05029600	1.56931200
C	4.52216200	1.72680500	1.93175000
C	3.61206300	0.76067000	1.46329800
C	2.45284900	2.43580100	0.27353800
C	3.31036600	3.41891700	0.72617100
H	5.08880400	3.79863900	1.93236400
H	5.33265300	1.41947100	2.58798600
H	1.62827400	2.67690200	-0.39811700
F	3.09398500	-4.64415900	2.73153600
F	5.47571900	-0.66385800	3.22175000
N	2.60023200	1.14954800	0.60903300
C	3.11514500	4.84666300	0.32801900
F	4.20379400	5.34239900	-0.27396600
F	2.88136800	5.62591200	1.39223500
F	2.08768500	4.99993100	-0.51200400
C	-2.99550000	3.27650600	-3.16559200
C	-4.08531100	3.77170900	-2.21464800
H	-3.67665800	4.43753500	-1.43856000
H	-4.83189800	4.34585700	-2.78255000
H	-4.59982700	2.93453300	-1.72255700
C	-2.30181600	4.48436400	-3.81288900
H	-3.04515100	5.09894400	-4.34331800
H	-1.81500600	5.11577400	-3.05373100
H	-1.53878900	4.17883100	-4.54435700
C	-3.64455300	2.40070600	-4.24891100
H	-2.90906400	2.04587900	-4.98622900
H	-4.13372600	1.52828100	-3.79402700
H	-4.40418200	2.98537100	-4.79027900
H	-2.87493100	2.11890300	1.45344300
C	-3.23686400	1.44261100	4.12376300
C	-3.99746600	0.13606200	4.40939400
H	-3.35252400	-0.61160900	4.89538700

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 H                -4.84552900    0.33968700    5.08157600
 H                -4.38873700   -0.29487500    3.47598000
 C                -2.67746500    2.02633200    5.42738600
 H                -2.10800300    2.94901400    5.23649100
 H                -3.50608900    2.27220200    6.10857100
 H                -2.01844900    1.31915400    5.95205400
 C                -4.20593500    2.44710900    3.49926000
 H                -3.70431400    3.39516800    3.24987200
 H                -4.67444000    2.04770600    2.58840500
 H                -5.00783000    2.67300600    4.21725100
 P                -4.88222500   -0.23329700   -0.31956600
 F                -3.28196900   -0.50534700   -0.11459700
 F                -5.15951800   -0.75892500    1.19502900
 F                -4.69104100    1.29448300    0.26211700
 F                -6.46511700    0.05660000   -0.52110100
 F                -4.58137700    0.32513200   -1.82276900
 F                -5.06481200   -1.73368500   -0.89994200
-1 2
 Ir                1.40318200   -0.37401300   -0.05211600
 C                -0.83621300   -4.32254200   -1.66326200
 C                -1.42325800   -3.58895800   -0.60636400
 C                -0.80612500   -2.43002300   -0.17584200
 C                 0.92035700   -2.66529800   -1.77116200
 C                 0.32345900   -3.85285000   -2.23969600
 H                -1.29516200   -5.24572700   -2.02092400
 H                -1.23392000   -1.83910300    0.63346000
 H                 0.78848400   -4.39373200   -3.06024400
 C                 3.60478700   -0.06766700   -2.08876000
 C                 2.49998200   -0.80157100   -1.62365900
 C                 2.09553300   -2.01870600   -2.28646600
 C                 2.88512200   -2.45170800   -3.36931700
 C                 3.97132200   -1.73130600   -3.82551300
 C                 4.31557700   -0.53517100   -3.17555600
 H                 3.92221700    0.85650400   -1.60471600
 H                 4.54938600   -2.09222400   -4.67701800
 N                 0.33647300   -1.98930700   -0.71358300
 F                 2.59013300   -3.58864900   -4.00060800
 F                 5.36387400    0.14568600   -3.63227700
 C                -2.65984300   -4.09853100    0.06319600
 F                -3.09760200   -3.28073300    1.01799800
 F                -2.43208200   -5.29331600    0.63928700
 F                -3.65252900   -4.28943300   -0.81040100
 C                -2.09305600    1.09710400    3.18093000
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C	-1.03065800	0.28598200	3.60558600
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C	-1.06482600	1.07420000	0.98787300
C	-2.07131500	1.50583000	1.84824400
H	-0.96391600	-0.07423600	4.63264300
H	0.77890800	-0.73891000	3.01303500
C	-1.94722100	2.44650300	-2.43791500
C	-2.00613600	2.19029700	-1.06827900
C	-1.03373000	1.41025300	-0.44771800
C	0.07077600	1.12269000	-2.46202800
C	-0.86524200	1.88877600	-3.13348900
H	-2.83948700	2.56203400	-0.48055200
H	0.92004800	0.67759100	-2.98352900
H	-0.74099100	2.03755400	-4.20675500
N	-0.07403100	0.27505400	1.42216300
N	-0.00767100	0.89009300	-1.14571000
C	4.45031300	-1.31357400	2.66957400
C	4.29794600	-2.65101300	2.98754500
C	3.23564000	-3.35948100	2.41608600
C	2.34641900	-2.76344800	1.53945900
C	2.50583200	-1.40710400	1.21804500
C	3.56864500	-0.63987300	1.80627300
H	4.99543700	-3.13663800	3.67069400
H	1.54307700	-3.36409700	1.11142800
C	4.38231700	3.05029600	1.56931200
C	4.52216200	1.72680500	1.93175000
C	3.61206300	0.76067000	1.46329800
C	2.45284900	2.43580100	0.27353800
C	3.31036600	3.41891700	0.72617100
H	5.08880400	3.79863900	1.93236400
H	5.33265300	1.41947100	2.58798600
H	1.62827400	2.67690200	-0.39811700
F	3.09398500	-4.64415900	2.73153600
F	5.47571900	-0.66385800	3.22175000
N	2.60023200	1.14954800	0.60903300
C	3.11514500	4.84666300	0.32801900
F	4.20379400	5.34239900	-0.27396600
F	2.88136800	5.62591200	1.39223500
F	2.08768500	4.99993100	-0.51200400
C	-2.99550000	3.27650600	-3.16559200
C	-4.08531100	3.77170900	-2.21464800
H	-3.67665800	4.43753500	-1.43856000
H	-4.83189800	4.34585700	-2.78255000

H	-4.59982700	2.93453300	-1.72255700
C	-2.30181600	4.48436400	-3.81288900
H	-3.04515100	5.09894400	-4.34331800
H	-1.81500600	5.11577400	-3.05373100
H	-1.53878900	4.17883100	-4.54435700
C	-3.64455300	2.40070600	-4.24891100
H	-2.90906400	2.04587900	-4.98622900
H	-4.13372600	1.52828100	-3.79402700
H	-4.40418200	2.98537100	-4.79027900
H	-2.87493100	2.11890300	1.45344300
C	-3.23686400	1.44261100	4.12376300
C	-3.99746600	0.13606200	4.40939400
H	-3.35252400	-0.61160900	4.89538700
H	-4.84552900	0.33968700	5.08157600
H	-4.38873700	-0.29487500	3.47598000
C	-2.67746500	2.02633200	5.42738600
H	-2.10800300	2.94901400	5.23649100
H	-3.50608900	2.27220200	6.10857100
H	-2.01844900	1.31915400	5.95205400
C	-4.20593500	2.44710900	3.49926000
H	-3.70431400	3.39516800	3.24987200
H	-4.67444000	2.04770600	2.58840500
H	-5.00783000	2.67300600	4.21725100
P	-4.88222500	-0.23329700	-0.31956600
F	-3.28196900	-0.50534700	-0.11459700
F	-5.15951800	-0.75892500	1.19502900
F	-4.69104100	1.29448300	0.26211700
F	-6.46511700	0.05660000	-0.52110100
F	-4.58137700	0.32513200	-1.82276900
F	-5.06481200	-1.73368500	-0.89994200

SET5

^{3}Ea-^{2}Sa

0 3

C	1.28194300	-1.26522300	0.25377000
C	1.97503900	-1.45379000	1.60030100
H	1.53066400	-0.80416300	2.36832000
H	1.85773000	-2.49775300	1.92546000
H	3.04861500	-1.23188000	1.53361000
C	1.93829800	-2.17872700	-0.79969800
H	1.82861100	-3.23304600	-0.50547400
H	1.47280800	-2.03860700	-1.78636200
H	3.00918300	-1.95769300	-0.88635500

C	2.37147900	1.18537200	-0.23452300
N	-0.06760600	-1.81051500	0.40599500
C	-1.08141200	-1.53976000	-0.46240200
H	-1.12778900	-2.16760600	-1.36382100
C	-2.14189400	-0.63742300	-0.18957500
C	-2.20941400	0.09798100	1.02601700
C	-3.18223500	-0.44146800	-1.13778400
C	-3.24646800	0.98906100	1.26014200
C	-4.21122600	0.45335500	-0.89026100
C	-4.25416600	1.18069700	0.30714400
H	-3.27747700	1.54155000	2.20303300
H	-4.99645900	0.59090100	-1.63836400
C	1.17697900	0.20306900	-0.22004100
H	0.39282200	0.68227700	0.38886100
H	0.76320700	0.16124200	-1.24177500
C	1.88806100	2.40717000	-1.02914200
H	2.66096400	3.19175300	-1.04796400
H	1.65274300	2.13736000	-2.07093600
H	0.97920200	2.83890900	-0.58008000
C	2.74370600	1.66653100	1.17251800
H	1.86043700	2.05650800	1.70314600
H	3.18515300	0.87289800	1.78916100
H	3.48260600	2.48122800	1.10877700
C	3.61504900	0.62560900	-0.92733700
H	4.07979600	-0.18796000	-0.35080000
H	3.38037600	0.24392400	-1.93330000
H	4.37283800	1.41751700	-1.03866500
H	-3.15767400	-1.00254800	-2.07587600
H	-5.06780700	1.88412400	0.49707300
H	-1.43973400	-0.06005700	1.78558700

1 2

C	1.28194300	-1.26522300	0.25377000
C	1.97503900	-1.45379000	1.60030100
H	1.53066400	-0.80416300	2.36832000
H	1.85773000	-2.49775300	1.92546000
H	3.04861500	-1.23188000	1.53361000
C	1.93829800	-2.17872700	-0.79969800
H	1.82861100	-3.23304600	-0.50547400
H	1.47280800	-2.03860700	-1.78636200
H	3.00918300	-1.95769300	-0.88635500
C	2.37147900	1.18537200	-0.23452300
N	-0.06760600	-1.81051500	0.40599500
C	-1.08141200	-1.53976000	-0.46240200

H	-1.12778900	-2.16760600	-1.36382100
C	-2.14189400	-0.63742300	-0.18957500
C	-2.20941400	0.09798100	1.02601700
C	-3.18223500	-0.44146800	-1.13778400
C	-3.24646800	0.98906100	1.26014200
C	-4.21122600	0.45335500	-0.89026100
C	-4.25416600	1.18069700	0.30714400
H	-3.27747700	1.54155000	2.20303300
H	-4.99645900	0.59090100	-1.63836400
C	1.17697900	0.20306900	-0.22004100
H	0.39282200	0.68227700	0.38886100
H	0.76320700	0.16124200	-1.24177500
C	1.88806100	2.40717000	-1.02914200
H	2.66096400	3.19175300	-1.04796400
H	1.65274300	2.13736000	-2.07093600
H	0.97920200	2.83890900	-0.58008000
C	2.74370600	1.66653100	1.17251800
H	1.86043700	2.05650800	1.70314600
H	3.18515300	0.87289800	1.78916100
H	3.48260600	2.48122800	1.10877700
C	3.61504900	0.62560900	-0.92733700
H	4.07979600	-0.18796000	-0.35080000
H	3.38037600	0.24392400	-1.93330000
H	4.37283800	1.41751700	-1.03866500
H	-3.15767400	-1.00254800	-2.07587600
H	-5.06780700	1.88412400	0.49707300
H	-1.43973400	-0.06005700	1.78558700

Ir(III)*-Ir(II)

0 3

Ir	1.40318200	-0.37401300	-0.05211600
C	-0.83621300	-4.32254200	-1.66326200
C	-1.42325800	-3.58895800	-0.60636400
C	-0.80612500	-2.43002300	-0.17584200
C	0.92035700	-2.66529800	-1.77116200
C	0.32345900	-3.85285000	-2.23969600
H	-1.29516200	-5.24572700	-2.02092400
H	-1.23392000	-1.83910300	0.63346000
H	0.78848400	-4.39373200	-3.06024400
C	3.60478700	-0.06766700	-2.08876000
C	2.49998200	-0.80157100	-1.62365900
C	2.09553300	-2.01870600	-2.28646600
C	2.88512200	-2.45170800	-3.36931700

C	3.97132200	-1.73130600	-3.82551300
C	4.31557700	-0.53517100	-3.17555600
H	3.92221700	0.85650400	-1.60471600
H	4.54938600	-2.09222400	-4.67701800
N	0.33647300	-1.98930700	-0.71358300
F	2.59013300	-3.58864900	-4.00060800
F	5.36387400	0.14568600	-3.63227700
C	-2.65984300	-4.09853100	0.06319600
F	-3.09760200	-3.28073300	1.01799800
F	-2.43208200	-5.29331600	0.63928700
F	-3.65252900	-4.28943300	-0.81040100
C	-2.09305600	1.09710400	3.18093000
C	-1.03065800	0.28598200	3.60558600
C	-0.04906400	-0.09586500	2.70892700
C	-1.06482600	1.07420000	0.98787300
C	-2.07131500	1.50583000	1.84824400
H	-0.96391600	-0.07423600	4.63264300
H	0.77890800	-0.73891000	3.01303500
C	-1.94722100	2.44650300	-2.43791500
C	-2.00613600	2.19029700	-1.06827900
C	-1.03373000	1.41025300	-0.44771800
C	0.07077600	1.12269000	-2.46202800
C	-0.86524200	1.88877600	-3.13348900
H	-2.83948700	2.56203400	-0.48055200
H	0.92004800	0.67759100	-2.98352900
H	-0.74099100	2.03755400	-4.20675500
N	-0.07403100	0.27505400	1.42216300
N	-0.00767100	0.89009300	-1.14571000
C	4.45031300	-1.31357400	2.66957400
C	4.29794600	-2.65101300	2.98754500
C	3.23564000	-3.35948100	2.41608600
C	2.34641900	-2.76344800	1.53945900
C	2.50583200	-1.40710400	1.21804500
C	3.56864500	-0.63987300	1.80627300
H	4.99543700	-3.13663800	3.67069400
H	1.54307700	-3.36409700	1.11142800
C	4.38231700	3.05029600	1.56931200
C	4.52216200	1.72680500	1.93175000
C	3.61206300	0.76067000	1.46329800
C	2.45284900	2.43580100	0.27353800
C	3.31036600	3.41891700	0.72617100
H	5.08880400	3.79863900	1.93236400
H	5.33265300	1.41947100	2.58798600

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H                1.62827400    2.67690200   -0.39811700
F                3.09398500   -4.64415900    2.73153600
F                5.47571900   -0.66385800    3.22175000
N                2.60023200    1.14954800    0.60903300
C                3.11514500    4.84666300    0.32801900
F                4.20379400    5.34239900   -0.27396600
F                2.88136800    5.62591200    1.39223500
F                2.08768500    4.99993100   -0.51200400
C               -2.99550000    3.27650600   -3.16559200
C               -4.08531100    3.77170900   -2.21464800
H               -3.67665800    4.43753500   -1.43856000
H               -4.83189800    4.34585700   -2.78255000
H               -4.59982700    2.93453300   -1.72255700
C               -2.30181600    4.48436400   -3.81288900
H               -3.04515100    5.09894400   -4.34331800
H               -1.81500600    5.11577400   -3.05373100
H               -1.53878900    4.17883100   -4.54435700
C               -3.64455300    2.40070600   -4.24891100
H               -2.90906400    2.04587900   -4.98622900
H               -4.13372600    1.52828100   -3.79402700
H               -4.40418200    2.98537100   -4.79027900
H               -2.87493100    2.11890300    1.45344300
C               -3.23686400    1.44261100    4.12376300
C               -3.99746600    0.13606200    4.40939400
H               -3.35252400   -0.61160900    4.89538700
H               -4.84552900    0.33968700    5.08157600
H               -4.38873700   -0.29487500    3.47598000
C               -2.67746500    2.02633200    5.42738600
H               -2.10800300    2.94901400    5.23649100
H               -3.50608900    2.27220200    6.10857100
H               -2.01844900    1.31915400    5.95205400
C               -4.20593500    2.44710900    3.49926000
H               -3.70431400    3.39516800    3.24987200
H               -4.67444000    2.04770600    2.58840500
H               -5.00783000    2.67300600    4.21725100
P               -4.88222500   -0.23329700   -0.31956600
F               -3.28196900   -0.50534700   -0.11459700
F               -5.15951800   -0.75892500    1.19502900
F               -4.69104100    1.29448300    0.26211700
F               -6.46511700    0.05660000   -0.52110100
F               -4.58137700    0.32513200   -1.82276900
F               -5.06481200   -1.73368500   -0.89994200
-1 2
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Ir	1.40318200	-0.37401300	-0.05211600
C	-0.83621300	-4.32254200	-1.66326200
C	-1.42325800	-3.58895800	-0.60636400
C	-0.80612500	-2.43002300	-0.17584200
C	0.92035700	-2.66529800	-1.77116200
C	0.32345900	-3.85285000	-2.23969600
H	-1.29516200	-5.24572700	-2.02092400
H	-1.23392000	-1.83910300	0.63346000
H	0.78848400	-4.39373200	-3.06024400
C	3.60478700	-0.06766700	-2.08876000
C	2.49998200	-0.80157100	-1.62365900
C	2.09553300	-2.01870600	-2.28646600
C	2.88512200	-2.45170800	-3.36931700
C	3.97132200	-1.73130600	-3.82551300
C	4.31557700	-0.53517100	-3.17555600
H	3.92221700	0.85650400	-1.60471600
H	4.54938600	-2.09222400	-4.67701800
N	0.33647300	-1.98930700	-0.71358300
F	2.59013300	-3.58864900	-4.00060800
F	5.36387400	0.14568600	-3.63227700
C	-2.65984300	-4.09853100	0.06319600
F	-3.09760200	-3.28073300	1.01799800
F	-2.43208200	-5.29331600	0.63928700
F	-3.65252900	-4.28943300	-0.81040100
C	-2.09305600	1.09710400	3.18093000
C	-1.03065800	0.28598200	3.60558600
C	-0.04906400	-0.09586500	2.70892700
C	-1.06482600	1.07420000	0.98787300
C	-2.07131500	1.50583000	1.84824400
H	-0.96391600	-0.07423600	4.63264300
H	0.77890800	-0.73891000	3.01303500
C	-1.94722100	2.44650300	-2.43791500
C	-2.00613600	2.19029700	-1.06827900
C	-1.03373000	1.41025300	-0.44771800
C	0.07077600	1.12269000	-2.46202800
C	-0.86524200	1.88877600	-3.13348900
H	-2.83948700	2.56203400	-0.48055200
H	0.92004800	0.67759100	-2.98352900
H	-0.74099100	2.03755400	-4.20675500
N	-0.07403100	0.27505400	1.42216300
N	-0.00767100	0.89009300	-1.14571000
C	4.45031300	-1.31357400	2.66957400
C	4.29794600	-2.65101300	2.98754500

C	3.23564000	-3.35948100	2.41608600
C	2.34641900	-2.76344800	1.53945900
C	2.50583200	-1.40710400	1.21804500
C	3.56864500	-0.63987300	1.80627300
H	4.99543700	-3.13663800	3.67069400
H	1.54307700	-3.36409700	1.11142800
C	4.38231700	3.05029600	1.56931200
C	4.52216200	1.72680500	1.93175000
C	3.61206300	0.76067000	1.46329800
C	2.45284900	2.43580100	0.27353800
C	3.31036600	3.41891700	0.72617100
H	5.08880400	3.79863900	1.93236400
H	5.33265300	1.41947100	2.58798600
H	1.62827400	2.67690200	-0.39811700
F	3.09398500	-4.64415900	2.73153600
F	5.47571900	-0.66385800	3.22175000
N	2.60023200	1.14954800	0.60903300
C	3.11514500	4.84666300	0.32801900
F	4.20379400	5.34239900	-0.27396600
F	2.88136800	5.62591200	1.39223500
F	2.08768500	4.99993100	-0.51200400
C	-2.99550000	3.27650600	-3.16559200
C	-4.08531100	3.77170900	-2.21464800
H	-3.67665800	4.43753500	-1.43856000
H	-4.83189800	4.34585700	-2.78255000
H	-4.59982700	2.93453300	-1.72255700
C	-2.30181600	4.48436400	-3.81288900
H	-3.04515100	5.09894400	-4.34331800
H	-1.81500600	5.11577400	-3.05373100
H	-1.53878900	4.17883100	-4.54435700
C	-3.64455300	2.40070600	-4.24891100
H	-2.90906400	2.04587900	-4.98622900
H	-4.13372600	1.52828100	-3.79402700
H	-4.40418200	2.98537100	-4.79027900
H	-2.87493100	2.11890300	1.45344300
C	-3.23686400	1.44261100	4.12376300
C	-3.99746600	0.13606200	4.40939400
H	-3.35252400	-0.61160900	4.89538700
H	-4.84552900	0.33968700	5.08157600
H	-4.38873700	-0.29487500	3.47598000
C	-2.67746500	2.02633200	5.42738600
H	-2.10800300	2.94901400	5.23649100
H	-3.50608900	2.27220200	6.10857100

H	-2.01844900	1.31915400	5.95205400
C	-4.20593500	2.44710900	3.49926000
H	-3.70431400	3.39516800	3.24987200
H	-4.67444000	2.04770600	2.58840500
H	-5.00783000	2.67300600	4.21725100
P	-4.88222500	-0.23329700	-0.31956600
F	-3.28196900	-0.50534700	-0.11459700
F	-5.15951800	-0.75892500	1.19502900
F	-4.69104100	1.29448300	0.26211700
F	-6.46511700	0.05660000	-0.52110100
F	-4.58137700	0.32513200	-1.82276900
F	-5.06481200	-1.73368500	-0.89994200

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Zero-point correction= 0.347901
Thermal correction to Energy= 0.361558
Thermal correction to Enthalpy= 0.362502
Thermal correction to Gibbs Free Energy= 0.306312
Sum of electronic and zero-point Energies= -713.581865
Sum of electronic and thermal Energies= -713.568207
Sum of electronic and thermal Enthalpies= -713.567263
Sum of electronic and thermal Free Energies= -713.623453

Cartesian coordinates

C	-1.904263	1.170471	-1.248875
H	-0.943594	1.707354	-1.268128
H	-2.459132	1.455746	-2.158757
C	-2.701870	1.558517	-0.000129
H	-2.881989	2.646542	-0.000206
C	-1.656200	-0.340220	-1.252439
H	-1.072736	-0.624271	-2.144217
C	-0.858083	-0.752962	0.000018
H	-0.764089	-1.860092	0.000098
C	-1.904238	1.170650	1.248656
H	-2.459087	1.456057	2.158509
H	-0.943566	1.707532	1.267810
C	-1.656178	-0.340041	1.252430
H	-1.072697	-0.623965	2.144238
C	-2.995353	-1.082658	1.247570
H	-2.827240	-2.172879	1.269433
H	-3.563397	-0.826825	2.157922
C	-4.042408	0.815386	-0.000063
H	-4.633975	1.100541	-0.886930

H	-4.633960	1.100667	0.886773
C	-2.995376	-1.082837	-1.247446
H	-3.563436	-0.827135	-2.157825
H	-2.827264	-2.173061	-1.269156
C	-3.794928	-0.696667	0.000042
H	-4.759744	-1.230594	0.000088
N	0.442848	-0.136954	-0.000029
C	1.466867	-0.886444	0.000079
H	1.371713	-1.992057	0.000193
C	2.844189	-0.370426	0.000047
C	3.107607	1.008152	-0.000125
C	3.917512	-1.270654	0.000203
C	4.418027	1.471670	-0.000140
H	2.262951	1.700395	-0.000245
C	5.231565	-0.805350	0.000190
H	3.716737	-2.345799	0.000338
C	5.483814	0.566152	0.000019
H	4.615764	2.546385	-0.000275
H	6.061693	-1.515596	0.000315
H	6.513008	0.933288	0.000009

Vibrational frequencies

26.3521	40.1273	56.3564
104.3815	151.3458	210.0202
277.1846	302.3070	326.3743
346.5222	381.2380	415.6698
420.6453	426.3384	445.9638
450.2930	467.9533	538.8157
561.2096	627.4652	636.7934
652.0357	671.2298	705.7149
720.0953	786.6434	790.9850
822.7216	831.7690	843.3175

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Zero-point correction= 0.346506

Thermal correction to Energy= 0.360530

Thermal correction to Enthalpy= 0.361474

Thermal correction to Gibbs Free Energy= 0.303965

Sum of electronic and zero-point Energies= -713.355045

Sum of electronic and thermal Energies= -713.341021

Sum of electronic and thermal Enthalpies= -713.340077

Sum of electronic and thermal Free Energies= -713.397586

Cartesian coordinates

C	1.734167	-1.387512	0.923376
H	0.709392	-1.573183	1.283141
H	2.316849	-2.285167	1.186855
C	2.324042	-0.148773	1.601767
H	2.296116	-0.284785	2.693978
C	1.774564	-1.224582	-0.591671
H	1.335402	-2.094165	-1.104036
C	0.955821	0.053334	-1.034940
H	1.064484	0.187946	-2.124650
C	1.488420	1.076729	1.218790
H	1.882333	1.977597	1.715577
H	0.447213	0.957438	1.561513
C	1.539086	1.291431	-0.292700
H	0.936466	2.164000	-0.585893
C	2.982076	1.467334	-0.761999
H	3.013752	1.635742	-1.850913
H	3.397417	2.369537	-0.285241
C	3.771246	0.046970	1.138558
H	4.379628	-0.826348	1.425717
H	4.212043	0.925488	1.637551
C	3.208620	-0.991311	-1.069419
H	3.791781	-1.894734	-0.824963
H	3.236005	-0.878682	-2.164754
C	3.807076	0.236456	-0.381119
H	4.846456	0.371361	-0.718463
N	-0.392287	-0.123321	-0.769155
C	-1.383217	-0.835057	-0.478471
H	-1.209006	-1.928531	-0.419197
C	-2.726261	-0.346330	-0.216861
C	-3.016829	1.029390	-0.245152
C	-3.732063	-1.280477	0.074288
C	-4.308685	1.458922	0.017752
H	-2.226274	1.748932	-0.470885
C	-5.024708	-0.838899	0.334772
H	-3.497942	-2.347192	0.094708
C	-5.310991	0.526164	0.306578
H	-4.542134	2.525179	-0.000895
H	-5.811315	-1.560961	0.561225
H	-6.326835	0.871029	0.512399

Vibrational frequencies

31.4283	33.1647	50.3454

107.9486 152.3005 210.4877
242.0787 269.8690 312.2183
322.9005 386.3781 388.3823
412.3697 416.2056 442.9511
450.5971 464.9346 476.7945
548.7283 624.0028 633.0204
634.9039 652.7092 689.0406
703.7763 767.8282 776.9380
803.1397 827.4782 832.9003

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Zero-point correction= 0.344314
Thermal correction to Energy= 0.358245
Thermal correction to Enthalpy= 0.359189
Thermal correction to Gibbs Free Energy= 0.299475
Sum of electronic and zero-point Energies= -713.499659
Sum of electronic and thermal Energies= -713.485727
Sum of electronic and thermal Enthalpies= -713.484783
Sum of electronic and thermal Free Energies= -713.544497

Cartesian coordinates

C	0.932743	1.338179	0.427291
H	0.024640	1.544372	-0.156651
H	0.928823	2.039347	1.278994
C	2.177086	1.557426	-0.436200
H	2.179019	2.590041	-0.821848
C	0.915911	-0.098722	0.958178
H	0.009954	-0.274226	1.561143
C	0.932994	-1.106583	-0.213101
H	1.006109	-2.118568	0.241637
C	2.154923	0.571871	-1.607533
H	3.022544	0.739956	-2.266804
H	1.248833	0.727180	-2.217251
C	2.174644	-0.864507	-1.078489
H	2.155146	-1.576845	-1.919459
C	3.421938	-1.091066	-0.220329
H	3.444465	-2.130948	0.149466
H	4.327702	-0.950076	-0.835167
C	3.429827	1.322940	0.414722
H	3.458689	2.042817	1.249709
H	4.336832	1.494009	-0.190116
C	2.170595	-0.335688	1.805924
H	2.166233	0.354880	2.666900

H	2.166411	-1.360183	2.215505
C	3.424833	-0.110227	0.954743
H	4.322211	-0.278012	1.572902
N	-0.264716	-1.142931	-1.006982
C	-1.452611	-1.501316	-0.435301
H	-1.574408	-2.580098	-0.253922
C	-2.556169	-0.641225	-0.212429
C	-2.561395	0.720563	-0.625933
C	-3.726737	-1.137738	0.425942
C	-3.656868	1.534624	-0.379453
H	-1.698724	1.112788	-1.168418
C	-4.814202	-0.312911	0.664813
H	-3.755855	-2.186151	0.737451
C	-4.789640	1.033181	0.271867
H	-3.635588	2.576285	-0.710225
H	-5.698399	-0.718337	1.163333
H	-5.648863	1.679467	0.463419

Vibrational frequencies

1.5729	43.4736	79.0984
120.1531	155.9088	206.3386
254.3711	295.0073	325.0306
340.4781	372.6037	407.2233
416.8304	423.8501	446.4403
451.1939	492.6134	502.8908
547.8284	601.9258	624.7489
645.6046	650.1920	671.4980
692.5358	701.2020	768.8262
786.3968	819.2316	830.3355

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Zero-point correction= 0.333144
Thermal correction to Energy= 0.352890
Thermal correction to Enthalpy= 0.353834
Thermal correction to Gibbs Free Energy= 0.284533
Sum of electronic and zero-point Energies= -824.676540
Sum of electronic and thermal Energies= -824.656793
Sum of electronic and thermal Enthalpies= -824.655849
Sum of electronic and thermal Free Energies= -824.725151

Cartesian coordinates

C	2.334094	1.331117	0.001407
C	2.949181	0.074059	0.004210

C	2.185333	-1.094260	0.000336
C	0.785920	-1.004742	-0.005079
C	0.124915	0.247523	-0.006805
C	0.944716	1.409872	-0.004232
C	-1.327359	0.435847	-0.013934
N	-2.205103	-0.487691	0.016983
C	-3.627637	-0.159915	0.006765
C	-4.221538	-0.878996	-1.209461
C	-3.978023	1.327727	-0.061735
O	0.016561	-2.098978	-0.011518
C	0.610048	-3.372579	-0.016316
C	-4.212285	-0.761923	1.289343
O	4.292307	0.081810	0.010692
C	4.985694	-1.142930	0.014769
O	0.296679	2.589567	-0.005887
C	1.035001	3.786237	-0.007167
H	2.968684	2.214922	0.004873
H	2.668483	-2.066979	0.001463
H	-1.610909	1.498805	-0.047352
H	-3.975830	-1.950695	-1.175471
H	-5.316670	-0.768373	-1.235316
H	-3.809566	-0.463486	-2.142283
H	-5.071214	1.449091	-0.068302
H	-3.587031	1.881736	0.805908
H	-3.585134	1.798615	-0.976404
H	1.232508	-3.531496	-0.912801
H	1.225734	-3.541313	0.883029
H	-0.214548	-4.095855	-0.023228
H	-3.795827	-0.258283	2.175584
H	-5.307500	-0.651853	1.311304
H	-3.963810	-1.831462	1.355875
H	6.054216	-0.896502	0.020732
H	4.750039	-1.739832	0.911507
H	4.760155	-1.740112	-0.884372
H	1.671354	3.869361	-0.903660
H	0.302661	4.602482	-0.010713
H	1.667187	3.873655	0.891846

Vibrational frequencies

12.6124	35.3792	64.4666
77.4392	89.2776	105.1916
115.6231	175.6537	182.1356
182.7056	187.7979	206.9912

234.0963 235.9143 249.6986
253.6984 273.2317 287.6674
290.8479 313.4766 325.7391
349.4480 356.6312 376.6866
394.5320 445.4084 473.1540
486.1064 516.1144 542.8041

36^{+}

Zero-point correction= 0.332743
Thermal correction to Energy= 0.352728
Thermal correction to Enthalpy= 0.353672
Thermal correction to Gibbs Free Energy= 0.283396
Sum of electronic and zero-point Energies= -824.469322
Sum of electronic and thermal Energies= -824.449338
Sum of electronic and thermal Enthalpies= -824.448394
Sum of electronic and thermal Free Energies= -824.518670

Cartesian coordinates

C	2.359914	1.307499	0.014955
C	2.917167	0.002000	0.073161
C	2.119194	-1.154867	0.008222
C	0.746575	-1.018613	-0.108739
C	0.125907	0.298460	-0.088310
C	0.998376	1.456703	-0.088224
C	-1.288933	0.527888	-0.045755
N	-2.156907	-0.399758	0.175785
C	-3.580614	-0.130803	0.105761
C	-4.107591	-1.081901	-0.981823
C	-3.974210	1.308173	-0.218695
O	-0.071910	-2.030674	-0.247396
C	0.423215	-3.358646	-0.235948
C	-4.151453	-0.548486	1.467272
O	4.221145	-0.030562	0.172534
C	4.925194	-1.265038	0.238468
O	0.376753	2.622528	-0.152731
C	1.130465	3.820602	-0.110059
H	3.045117	2.151429	0.057722
H	2.576878	-2.139637	0.015763
H	-1.577548	1.578907	-0.185920
H	-3.822653	-2.119571	-0.757936
H	-5.204605	-1.015712	-1.028028
H	-3.698463	-0.810747	-1.966356
H	-5.070002	1.387497	-0.249879

H	-3.613724	2.012478	0.546962
H	-3.589022	1.627242	-1.199273
H	1.113293	-3.522016	-1.077854
H	0.932318	-3.576533	0.714925
H	-0.452518	-4.006419	-0.345018
H	-3.772969	0.108993	2.264157
H	-5.249032	-0.478064	1.449676
H	-3.865495	-1.583290	1.703243
H	5.982929	-1.000879	0.334041
H	4.605447	-1.845252	1.115999
H	4.769339	-1.846965	-0.681347
H	1.829712	3.871972	-0.958884
H	0.405924	4.638486	-0.180391
H	1.686271	3.898216	0.836933

Vibrational frequencies

19.3421	28.4693	49.9627
82.4688	94.8730	112.3728
138.2645	167.4546	168.9594
171.1559	181.9665	205.8593
223.0226	232.1907	234.5174
246.5144	253.2532	277.5864
281.4830	314.6403	316.5443
349.3545	352.5457	365.5949
398.9084	441.3115	455.9126
479.1944	491.9471	510.6546

^{3}36

Zero-point correction= 0.330101
Thermal correction to Energy= 0.350034
Thermal correction to Enthalpy= 0.350978
Thermal correction to Gibbs Free Energy= 0.281430
Sum of electronic and zero-point Energies= -824.601684
Sum of electronic and thermal Energies= -824.581751
Sum of electronic and thermal Enthalpies= -824.580806
Sum of electronic and thermal Free Energies= -824.650355

Cartesian coordinates

C	2.453396	1.078281	-0.061048
C	2.765722	-0.290700	-0.101430
C	1.762708	-1.251433	0.065132
C	0.443760	-0.840755	0.273283
C	0.080525	0.536445	0.325150

C	1.143728	1.481292	0.147503
C	-1.236439	1.003340	0.544390
N	-2.337164	0.241538	0.818604
C	-3.323039	-0.065174	-0.212924
C	-4.085610	-1.307527	0.241852
C	-2.695487	-0.291178	-1.588778
O	-0.572294	-1.714073	0.436311
C	-0.309632	-3.092886	0.412799
C	-4.270989	1.145068	-0.261062
O	4.066890	-0.589611	-0.308678
C	4.450137	-1.939002	-0.368064
O	0.765091	2.774698	0.197206
C	1.735749	3.777363	0.037995
H	3.263182	1.793043	-0.198153
H	2.001820	-2.311346	0.031647
H	-1.379887	2.089287	0.613568
H	-4.523368	-1.145821	1.238079
H	-4.894815	-1.548686	-0.463647
H	-3.405601	-2.169934	0.300829
H	-3.476398	-0.529096	-2.326580
H	-2.158814	0.607493	-1.928022
H	-1.981125	-1.125369	-1.550416
H	0.108224	-3.411860	-0.557051
H	0.384658	-3.388530	1.217301
H	-1.271398	-3.597043	0.568509
H	-3.735515	2.049680	-0.586637
H	-5.084706	0.949318	-0.975876
H	-4.713005	1.334910	0.728228
H	5.532844	-1.951762	-0.544337
H	4.236391	-2.467403	0.576914
H	3.947762	-2.471033	-1.194187
H	2.226745	3.714510	-0.947819
H	1.211065	4.737451	0.115505
H	2.507426	3.724514	0.824417

Vibrational frequencies

34.8102	44.0024	56.9434
69.1264	85.0319	114.2979
130.0561	159.6636	176.1964
190.0921	194.5860	208.1816
222.8038	246.5281	253.6260
273.1770	278.0977	287.8467
292.9739	295.6767	315.5156

354.0113 366.2778 374.6555
404.8588 427.0722 446.1530
485.1312 493.8764 536.3988

R1s

Zero-point correction= 0.446380
Thermal correction to Energy= 0.471246
Thermal correction to Enthalpy= 0.472190
Thermal correction to Gibbs Free Energy= 0.391734
Sum of electronic and zero-point Energies= -981.516629
Sum of electronic and thermal Energies= -981.491763
Sum of electronic and thermal Enthalpies= -981.490819
Sum of electronic and thermal Free Energies= -981.571275

Cartesian coordinates

C	-2.391184	0.494413	0.668358
C	-2.887018	0.102752	2.063118
H	-2.832922	-0.985856	2.206141
H	-2.247478	0.577205	2.823650
H	-3.920322	0.434498	2.236400
C	-2.523022	2.009539	0.500122
H	-1.890554	2.539447	1.229910
H	-2.234086	2.341530	-0.508765
H	-3.556931	2.331609	0.669795
C	-4.626765	-0.443103	-0.618392
N	-1.014298	-0.008245	0.604950
C	-0.055882	0.750213	0.246337
H	-0.216418	1.811462	0.003162
C	1.348631	0.353269	0.118413
C	1.826473	-0.978826	0.154564
C	2.310951	1.380274	-0.082285
C	3.189676	-1.270653	0.000306
C	3.665735	1.100787	-0.234073
C	4.099231	-0.229026	-0.190503
H	3.532033	-2.301066	0.028863
H	4.409731	1.880758	-0.382212
O	1.832078	2.638003	-0.109802
O	0.920417	-1.948891	0.326665
O	5.420772	-0.416005	-0.342552
C	1.328862	-3.293332	0.332409
H	0.419783	-3.890311	0.474978
H	1.801169	-3.582122	-0.621527
H	2.028468	-3.505578	1.158120

C	2.713182	3.710630	-0.333876
H	3.221181	3.622062	-1.308440
H	2.101364	4.620753	-0.329841
H	3.472641	3.784490	0.461951
C	5.937511	-1.724737	-0.314985
H	5.518552	-2.343738	-1.125688
H	7.021074	-1.635307	-0.458007
H	5.742818	-2.218238	0.651729
C	-3.094758	-0.277617	-0.479383
H	-2.664951	-1.293033	-0.462387
H	-2.720672	0.181169	-1.411736
C	-4.857195	-1.006136	-2.027880
H	-5.926095	-1.211769	-2.197727
H	-4.520948	-0.295824	-2.799984
H	-4.304375	-1.948183	-2.173224
C	-5.188327	-1.459929	0.382282
H	-4.639060	-2.413254	0.324371
H	-5.137372	-1.104280	1.419484
H	-6.246789	-1.668402	0.157291
C	-5.403988	0.869365	-0.498167
H	-5.375564	1.276383	0.523517
H	-5.009627	1.635945	-1.183438
H	-6.463392	0.705210	-0.753729

Vibrational frequencies

15.2254	26.8410	35.5412
41.2142	73.2788	80.4800
97.7502	115.5590	121.4454
161.2813	176.2248	184.6875
188.2560	203.9636	210.8784
223.0732	236.0012	249.1355
259.5015	271.3257	276.6530
281.2730	288.5390	291.3939
310.5052	319.6743	321.9701
335.5635	349.8857	370.2432

R1^{+}

Zero-point correction= 0.445923

Thermal correction to Energy= 0.471020

Thermal correction to Enthalpy= 0.471964

Thermal correction to Gibbs Free Energy= 0.390074

Sum of electronic and zero-point Energies= -981.309883

Sum of electronic and thermal Energies= -981.284786

Sum of electronic and thermal Enthalpies= -981.283842
Sum of electronic and thermal Free Energies= -981.365732

Cartesian coordinates

C	-2.354132	0.616144	0.716830
C	-2.873467	0.254815	2.110547
H	-2.786666	-0.824546	2.295135
H	-2.279365	0.783682	2.870992
H	-3.921700	0.557600	2.232204
C	-2.517652	2.114762	0.465891
H	-1.923109	2.697147	1.187062
H	-2.213148	2.399891	-0.552015
H	-3.564505	2.411505	0.593289
C	-4.492169	-0.481821	-0.591577
N	-0.972432	0.158234	0.699067
C	-0.011072	0.894732	0.254086
H	-0.148872	1.962635	0.032543
C	1.323802	0.421240	0.049077
C	1.705047	-0.981581	0.074866
C	2.365085	1.402123	-0.178478
C	3.038349	-1.353208	0.029823
C	3.683473	1.019919	-0.238281
C	4.018271	-0.355257	-0.123062
H	3.320790	-2.401129	0.075079
H	4.498513	1.729077	-0.366629
O	1.943129	2.652498	-0.272438
O	0.714698	-1.836848	0.138233
O	5.300647	-0.610911	-0.189516
C	0.973214	-3.227553	0.225085
H	-0.006774	-3.711995	0.283692
H	1.507435	-3.578066	-0.671166
H	1.559011	-3.459586	1.127095
C	2.884365	3.697234	-0.437930
H	3.454318	3.564260	-1.370320
H	2.304308	4.624402	-0.490563
H	3.574801	3.739708	0.418386
C	5.793303	-1.940642	-0.084271
H	5.411784	-2.560728	-0.908195
H	6.882671	-1.862473	-0.155285
H	5.514330	-2.380054	0.884202
C	-2.970654	-0.244333	-0.429867
H	-2.499226	-1.238840	-0.366438
H	-2.594692	0.203871	-1.365181

C	-4.654138	-1.101742	-1.987098
H	-5.708111	-1.359728	-2.175641
H	-4.329132	-0.403199	-2.774158
H	-4.057733	-2.022903	-2.083770
C	-5.030723	-1.489379	0.430067
H	-4.431627	-2.413755	0.426643
H	-5.037097	-1.094053	1.453795
H	-6.067917	-1.761145	0.177519
C	-5.324533	0.800066	-0.536160
H	-5.338391	1.244204	0.470085
H	-4.949855	1.557181	-1.242305
H	-6.369018	0.578371	-0.807052

Vibrational frequencies

10.9792	20.3211	30.6634
43.8405	85.8162	94.6771
111.0724	114.2794	138.8527
154.5496	163.2436	168.9806
179.0855	203.6507	207.6101
219.7950	226.2061	238.2160
251.6089	259.7133	270.3865
278.0369	280.5858	284.6382
309.7282	314.7887	317.6807
330.3115	354.9561	362.0155

R1t

Zero-point correction= 0.443523
Thermal correction to Energy= 0.468527
Thermal correction to Enthalpy= 0.469471
Thermal correction to Gibbs Free Energy= 0.388940
Sum of electronic and zero-point Energies= -981.442853
Sum of electronic and thermal Energies= -981.417848
Sum of electronic and thermal Enthalpies= -981.416904
Sum of electronic and thermal Free Energies= -981.497436

Cartesian coordinates

C	-2.447824	0.648167	0.964668
C	-3.176063	-0.322686	1.890629
H	-2.657052	-1.290640	1.928354
H	-3.194477	0.094514	2.908246
H	-4.212719	-0.490071	1.567690
C	-3.195315	1.994330	0.938831
H	-3.232254	2.424676	1.950762

H	-2.689541	2.709282	0.272722
H	-4.225453	1.861691	0.585124
C	-3.239371	-0.598716	-1.328048
N	-1.176986	0.958921	1.625821
C	-0.103158	1.462329	0.949292
H	-0.095157	2.551561	0.814512
C	1.054579	0.753045	0.551196
C	1.234046	-0.650349	0.723391
C	2.139621	1.460884	-0.061614
C	2.398978	-1.304821	0.316317
C	3.298015	0.816229	-0.466545
C	3.430137	-0.569527	-0.277591
H	2.498404	-2.377157	0.464316
H	4.123071	1.350981	-0.934472
O	1.938068	2.786045	-0.211319
O	0.199646	-1.298507	1.300292
O	4.592754	-1.111034	-0.702814
C	0.255842	-2.691867	1.459084
H	-0.692027	-2.991449	1.923091
H	0.358241	-3.207486	0.489122
H	1.087887	-2.994806	2.116848
C	2.948955	3.568429	-0.793102
H	3.168289	3.246700	-1.825180
H	2.576540	4.599946	-0.811435
H	3.880327	3.532111	-0.203173
C	4.794178	-2.491473	-0.544004
H	4.042567	-3.081148	-1.096507
H	5.788458	-2.713909	-0.950759
H	4.768431	-2.789363	0.518304
C	-2.173805	0.103855	-0.455249
H	-1.337606	-0.604728	-0.358200
H	-1.775443	0.955609	-1.032345
C	-2.618385	-0.708412	-2.727906
H	-3.288336	-1.251538	-3.413381
H	-2.427316	0.287875	-3.157360
H	-1.658654	-1.248775	-2.692551
C	-3.533081	-2.023136	-0.842222
H	-2.601173	-2.599532	-0.725047
H	-4.062378	-2.041924	0.119113
H	-4.164215	-2.550901	-1.575262
C	-4.550299	0.180813	-1.446217
H	-5.100025	0.215776	-0.493787
H	-4.374702	1.215959	-1.778735

H -5.210804 -0.300307 -2.185492

Vibrational frequencies

24.8490	29.6688	40.0285
59.8132	72.8639	79.6045
104.9667	113.8645	132.0269
156.7247	173.2385	183.5568
190.1681	205.1339	208.5129
236.8295	244.5356	245.6313
257.6621	263.9257	277.1981
280.4923	282.0548	293.9823
310.6643	316.7026	319.6946
328.6893	368.5459	371.7101

Ir01-acn

Zero-point correction= 0.709863
Thermal correction to Energy= 0.768320
Thermal correction to Enthalpy= 0.769264
Thermal correction to Gibbs Free Energy= 0.611566
Sum of electronic and zero-point Energies= -3876.609630
Sum of electronic and thermal Energies= -3876.551173
Sum of electronic and thermal Enthalpies= -3876.550228
Sum of electronic and thermal Free Energies= -3876.707926

Cartesian coordinates

Ir	1.354165	-0.379801	-0.057787
C	-1.270632	-3.826612	-2.154973
C	-1.671244	-3.328995	-0.914374
C	-0.923290	-2.318509	-0.333882
C	0.612315	-2.317768	-2.106553
C	-0.130741	-3.316057	-2.752470
H	-1.843299	-4.613039	-2.650351
H	-1.212482	-1.884828	0.621548
H	0.201874	-3.695800	-3.714404
C	3.666933	-0.182462	-2.039623
C	2.452500	-0.776649	-1.683773
C	1.863398	-1.727448	-2.564532
C	2.516409	-2.028211	-3.769401
C	3.715504	-1.438144	-4.130906
C	4.269082	-0.519743	-3.244770
H	4.162830	0.548413	-1.398857
H	4.200737	-1.688839	-5.073771
N	0.180269	-1.831069	-0.908725

F	1.988542	-2.908092	-4.622901
F	5.423336	0.054840	-3.574651
C	-2.839761	-3.926604	-0.184946
F	-3.271169	-3.143545	0.800787
F	-2.500506	-5.102493	0.366639
F	-3.859137	-4.170416	-1.008407
C	-2.165282	0.630922	3.256227
C	-1.106017	-0.219645	3.605420
C	-0.082025	-0.456141	2.704630
C	-1.030174	0.968359	1.142338
C	-2.091913	1.238870	2.003220
H	-1.077490	-0.726532	4.570701
H	0.738612	-1.136769	2.941426
C	-1.707732	2.983044	-2.002357
C	-1.817542	2.504378	-0.697454
C	-0.924594	1.553010	-0.209506
C	0.223116	1.552277	-2.221760
C	-0.644713	2.481954	-2.767486
H	-2.627085	2.843588	-0.059224
H	1.060127	1.149036	-2.795464
H	-0.483635	2.802242	-3.797385
N	-0.052893	0.107773	1.490939
N	0.087517	1.094577	-0.971137
C	4.372777	-1.833040	2.519569
C	4.213825	-3.204462	2.616373
C	3.181082	-3.781582	1.883735
C	2.325739	-3.041193	1.078684
C	2.488665	-1.655409	0.987368
C	3.538211	-1.034237	1.722793
H	4.874624	-3.801988	3.243791
H	1.540204	-3.568017	0.534677
C	4.555734	2.615661	1.922221
C	4.589148	1.254519	2.166320
C	3.636353	0.410601	1.574444
C	2.646621	2.260875	0.525990
C	3.563680	3.133486	1.085616
H	5.299602	3.271440	2.379174
H	5.352823	0.831083	2.812692
H	1.859080	2.618366	-0.136435
F	3.014623	-5.099373	1.964352
F	5.362637	-1.282124	3.225192
N	2.682810	0.944971	0.760412
C	3.490694	4.606333	0.805876

F	4.642658	5.061877	0.304440
F	3.251875	5.300926	1.922924
F	2.524699	4.901201	-0.065560
C	-2.705346	3.963382	-2.604652
C	-3.734450	4.431667	-1.575379
H	-3.258542	4.959373	-0.734173
H	-4.435089	5.132039	-2.053278
H	-4.317889	3.590016	-1.175312
C	-1.953436	5.182614	-3.155408
H	-2.669165	5.890950	-3.599802
H	-1.406938	5.705036	-2.355150
H	-1.231767	4.905574	-3.937922
C	-3.442548	3.237032	-3.742033
H	-2.751193	2.911498	-4.533817
H	-3.969312	2.352302	-3.355383
H	-4.181690	3.914059	-4.197702
H	-2.894635	1.884934	1.661344
C	-3.346853	0.828235	4.196383
C	-4.039742	-0.533563	4.369075
H	-3.366933	-1.279878	4.817563
H	-4.911586	-0.425277	5.032710
H	-4.385407	-0.913804	3.397078
C	-2.836358	1.335691	5.552064
H	-2.324021	2.304072	5.444226
H	-3.684619	1.472097	6.240024
H	-2.136955	0.628777	6.022415
C	-4.358973	1.827038	3.635076
H	-3.911813	2.823247	3.493641
H	-4.770255	1.487945	2.673835
H	-5.194316	1.935675	4.342428
P	-4.823845	-0.049325	-0.489177
F	-3.207573	-0.273558	-0.555342
F	-4.831120	-0.589257	1.047980
F	-4.589463	1.478795	0.065107
F	-6.429301	0.184408	-0.419572
F	-4.801389	0.515612	-2.017650
F	-5.055592	-1.557360	-1.039681

Vibrational frequencies

12.3877	13.4575	14.2068
17.6373	20.4135	25.0303
27.7894	30.7988	34.3808
34.5990	40.0148	50.8288

53.8380 56.3172 59.8490
62.0740 65.0422 67.4175
69.0349 73.1249 73.6923
75.7234 80.3053 83.9970
104.7065 121.1275 133.3711
140.5619 142.8454 145.4876

Ir-12-acn

Zero-point correction= 0.706418
Thermal correction to Energy= 0.765124
Thermal correction to Enthalpy= 0.766068
Thermal correction to Gibbs Free Energy= 0.606806
Sum of electronic and zero-point Energies= -3876.715681
Sum of electronic and thermal Energies= -3876.656974
Sum of electronic and thermal Enthalpies= -3876.656030
Sum of electronic and thermal Free Energies= -3876.815292

Cartesian coordinates

Ir	1.442371	-0.370887	-0.084509
C	-1.383684	-3.550987	-2.321115
C	-1.725316	-3.117564	-1.038358
C	-0.908032	-2.191223	-0.412264
C	0.575521	-2.142318	-2.229745
C	-0.235405	-3.058495	-2.917329
H	-2.010726	-4.270626	-2.851082
H	-1.141959	-1.802010	0.577844
H	0.048902	-3.384291	-3.914025
C	3.707308	-0.121410	-2.135091
C	2.480732	-0.691015	-1.771437
C	1.833809	-1.568644	-2.690426
C	2.439071	-1.818797	-3.930962
C	3.646927	-1.249689	-4.297332
C	4.259689	-0.405068	-3.375906
H	4.247078	0.553039	-1.467282
H	4.093934	-1.460011	-5.268552
N	0.205398	-1.725302	-0.986027
F	1.855027	-2.629703	-4.819254
F	5.425135	0.149054	-3.711462
C	-2.910649	-3.692424	-0.321194
F	-3.268646	-2.961749	0.731795
F	-2.637722	-4.927796	0.133475
F	-3.965196	-3.810185	-1.129177
C	-2.073759	0.325275	3.293301

C	-0.949594	-0.497193	3.614949
C	0.070452	-0.629448	2.698366
C	-0.951506	0.850315	1.186113
C	-2.042012	0.990568	2.088767
H	-0.890805	-1.047194	4.554462
H	0.923973	-1.283351	2.898457
C	-1.695685	3.042140	-1.788256
C	-1.815163	2.454388	-0.549197
C	-0.870013	1.502448	-0.077975
C	0.317494	1.733394	-2.090342
C	-0.572553	2.661771	-2.584423
H	-2.664233	2.688951	0.087167
H	1.182937	1.417222	-2.679138
H	-0.405641	3.077263	-3.578530
N	0.083845	-0.005229	1.510749
N	0.196885	1.160873	-0.883209
C	4.505875	-1.988876	2.345744
C	4.343825	-3.363245	2.368082
C	3.291617	-3.893773	1.625829
C	2.423144	-3.105949	0.884714
C	2.586352	-1.715043	0.867721
C	3.657582	-1.143014	1.615413
H	5.015609	-3.998023	2.945221
H	1.621595	-3.595690	0.328191
C	4.685828	2.490529	2.005500
C	4.723762	1.117463	2.169107
C	3.759792	0.307873	1.546423
C	2.750769	2.215092	0.623873
C	3.676672	3.054634	1.219410
H	5.437334	3.120109	2.486326
H	5.498060	0.657725	2.777134
H	1.944118	2.598865	-0.001100
F	3.122880	-5.216114	1.635908
F	5.516103	-1.482773	3.060407
N	2.794442	0.887861	0.778568
C	3.595038	4.540393	1.032787
F	4.738524	5.032867	0.543322
F	3.371862	5.167167	2.193689
F	2.615679	4.887191	0.195861
C	-2.717051	4.029386	-2.342389
C	-3.791428	4.383043	-1.313723
H	-3.354765	4.861939	-0.423237
H	-4.508411	5.091300	-1.756766

H	-4.347856	3.493406	-0.987050
C	-2.005211	5.319451	-2.773329
H	-2.735407	6.038146	-3.178006
H	-1.499043	5.793288	-1.917553
H	-1.251554	5.135504	-3.553191
C	-3.400062	3.381974	-3.557912
H	-2.670710	3.117196	-4.338398
H	-3.931772	2.467870	-3.254869
H	-4.130403	4.078428	-4.000741
H	-2.891014	1.592049	1.773589
C	-3.264776	0.385141	4.242985
C	-3.906991	-1.011239	4.290383
H	-3.191363	-1.773844	4.633516
H	-4.763784	-1.015228	4.983561
H	-4.267652	-1.299828	3.291781
C	-2.787065	0.784031	5.646024
H	-2.316217	1.779612	5.632265
H	-3.641056	0.820696	6.340863
H	-2.056960	0.069465	6.053841
C	-4.320021	1.389931	3.779863
H	-3.906648	2.408965	3.719538
H	-4.727546	1.122675	2.795211
H	-5.152862	1.408666	4.499779
P	-5.165758	0.051871	-0.449157
F	-3.583865	-0.303042	-0.580200
F	-5.215262	-0.664739	1.014140
F	-4.795371	1.477552	0.271576
F	-6.747227	0.416239	-0.320458
F	-5.120691	0.785420	-1.907035
F	-5.547573	-1.356322	-1.164267

Vibrational frequencies

7.6484	13.0645	16.0974
17.4376	18.3123	24.5810
29.3942	31.5555	34.4030
35.0929	35.8951	48.5532
49.2236	55.3744	58.0191
63.9925	64.7983	67.9803
72.6777	74.2139	74.7872
77.2748	80.9470	85.6625
102.6068	115.2109	135.9466
139.4122	144.0133	147.8728

Ir03-acn

Zero-point correction= 0.709519
Thermal correction to Energy= 0.768383
Thermal correction to Enthalpy= 0.769327
Thermal correction to Gibbs Free Energy= 0.609581
Sum of electronic and zero-point Energies= -3876.503268
Sum of electronic and thermal Energies= -3876.444404
Sum of electronic and thermal Enthalpies= -3876.443459
Sum of electronic and thermal Free Energies= -3876.603206

Cartesian coordinates

Ir	1.406984	-0.379010	-0.049503
C	-0.841874	-4.323105	-1.659098
C	-1.422282	-3.592075	-0.596928
C	-0.800098	-2.436446	-0.165259
C	0.917819	-2.669355	-1.769458
C	0.316701	-3.853610	-2.239079
H	-1.303454	-5.244442	-2.018203
H	-1.219367	-1.848155	0.650388
H	0.776836	-4.393169	-3.063236
C	3.606819	-0.077523	-2.089280
C	2.502251	-0.810213	-1.623639
C	2.093770	-2.022909	-2.287704
C	2.876624	-2.453600	-3.375156
C	3.964087	-1.734949	-3.833615
C	4.313016	-0.543668	-3.180700
H	3.926698	0.845464	-1.604653
H	4.537437	-2.094360	-4.688883
N	0.339947	-1.995868	-0.708296
F	2.575786	-3.587294	-4.009706
F	5.361296	0.137560	-3.637522
C	-2.658034	-4.098148	0.075253
F	-3.089286	-3.280807	1.034673
F	-2.438790	-5.296341	0.645659
F	-3.656984	-4.277874	-0.795553
C	-2.085014	1.110428	3.181612
C	-1.023929	0.298868	3.608261
C	-0.044536	-0.089271	2.711643
C	-1.061237	1.074138	0.986681
C	-2.065528	1.511800	1.846544
H	-0.954875	-0.055802	4.637050
H	0.782637	-0.732012	3.018243
C	-1.941048	2.441629	-2.441474

C	-2.001127	2.187231	-1.071504
C	-1.030828	1.405315	-0.449913
C	0.072516	1.110930	-2.463938
C	-0.861721	1.878378	-3.136652
H	-2.830807	2.566098	-0.483117
H	0.920840	0.663878	-2.985139
H	-0.736224	2.025656	-4.209973
N	-0.070999	0.275475	1.423178
N	-0.006274	0.881289	-1.147092
C	4.456708	-1.310001	2.669445
C	4.303988	-2.646402	2.990384
C	3.238982	-3.356435	2.423781
C	2.348061	-2.762639	1.548647
C	2.507339	-1.406375	1.223408
C	3.572400	-0.636914	1.807984
H	5.003274	-3.130989	3.672534
H	1.542871	-3.363532	1.124540
C	4.383962	3.052116	1.561907
C	4.524814	1.729917	1.927699
C	3.615240	0.761717	1.461789
C	2.454335	2.432658	0.267010
C	3.311270	3.417460	0.717442
H	5.089776	3.801787	1.923408
H	5.335429	1.425207	2.585006
H	1.630085	2.672092	-0.405532
F	3.098503	-4.640613	2.743712
F	5.484670	-0.660183	3.216471
N	2.602562	1.147590	0.605824
C	3.115547	4.843536	0.315175
F	4.202639	5.337394	-0.292299
F	2.886515	5.627390	1.377652
F	2.085546	4.995922	-0.521657
C	-2.984542	3.277036	-3.169941
C	-4.071387	3.780029	-2.219675
H	-3.658467	4.442659	-1.443261
H	-4.813627	4.359304	-2.788117
H	-4.591782	2.946530	-1.727353
C	-2.283674	4.480203	-3.818191
H	-3.023284	5.098625	-4.349392
H	-1.793370	5.108843	-3.059081
H	-1.522211	4.169128	-4.548854
C	-3.638759	2.404518	-4.252730
H	-2.905162	2.043748	-4.988971

H	-4.134138	1.535734	-3.797233
H	-4.394060	2.993579	-4.795416
H	-2.866320	2.128169	1.451038
C	-3.224876	1.465619	4.125789
C	-3.990821	0.164067	4.419894
H	-3.347586	-0.584585	4.906529
H	-4.835521	0.374348	5.094294
H	-4.387533	-0.269281	3.489714
C	-2.659673	2.052295	5.425538
H	-2.085457	2.970663	5.228632
H	-3.485610	2.305957	6.107159
H	-2.003423	1.343773	5.951691
C	-4.190567	2.472325	3.499515
H	-3.684776	3.416531	3.244450
H	-4.662874	2.071860	2.591021
H	-4.989608	2.705180	4.218499
P	-4.902860	-0.235345	-0.319094
F	-3.307573	-0.520595	-0.109358
F	-5.191845	-0.756572	1.195593
F	-4.703741	1.290666	0.258247
F	-6.484693	0.064880	-0.526523
F	-4.596320	0.313178	-1.824452
F	-5.098612	-1.737310	-0.895353

Vibrational frequencies

8.5945	14.7567	16.7419
19.7037	21.6695	26.5729
27.3398	30.4798	31.0519
35.6144	38.0529	48.7097
52.0542	55.2299	57.2080
60.8721	61.3427	65.2247
67.2315	71.0977	73.8071
76.5566	79.2253	83.5200
105.1834	124.0959	127.4672
139.1470	142.1673	142.8672