Electronic Supplementary Material (ESI) for RSC Advances.

Mechanistic insight into the selective cyclization of arylnitrones to indolines via Rh(III) catalyst: a theoretical study

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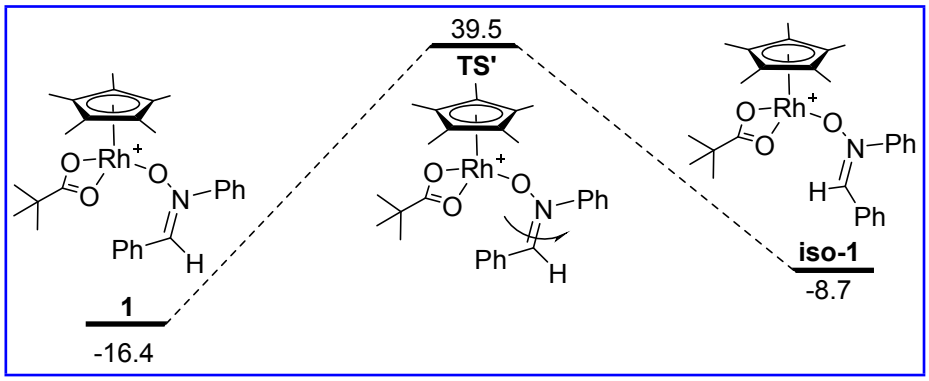


Fig. S1 The transformation from **1** to **iso-1**. Free energies (in kcal/mol) are relative to **cat-1**.

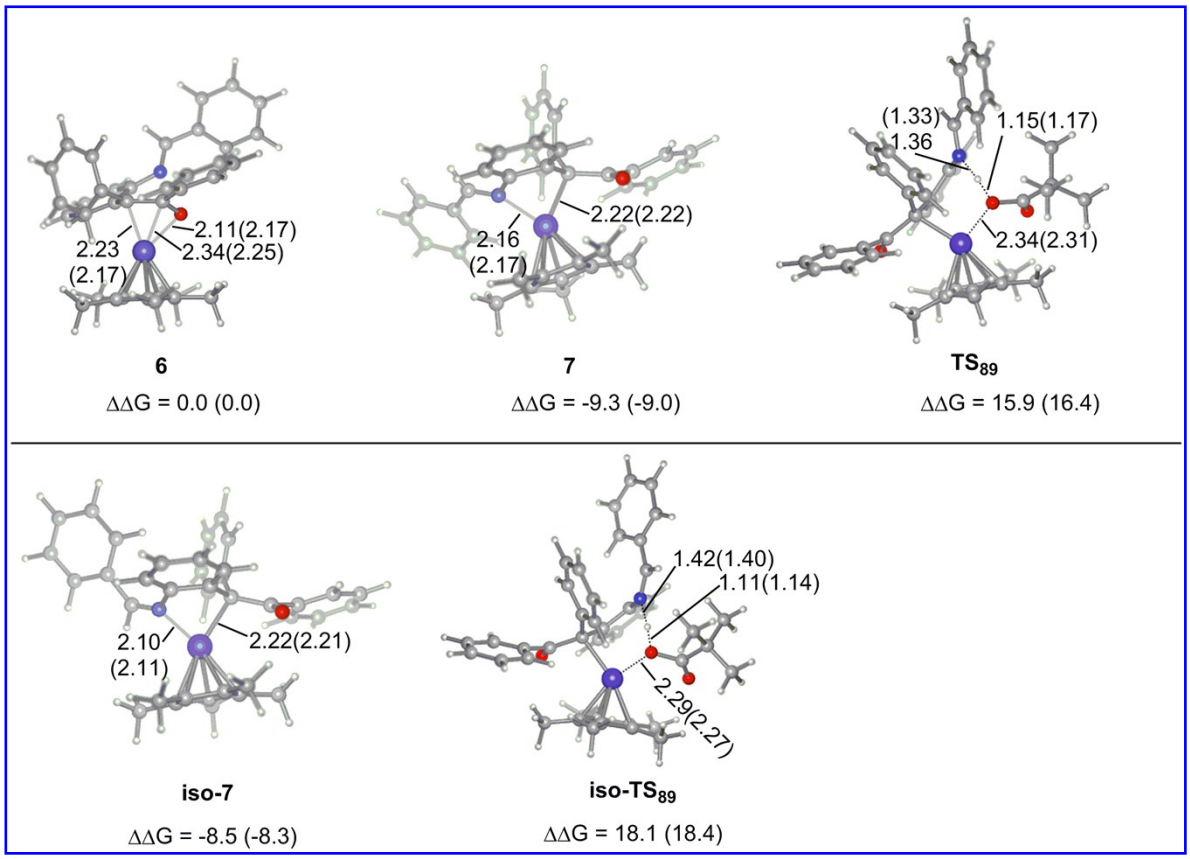
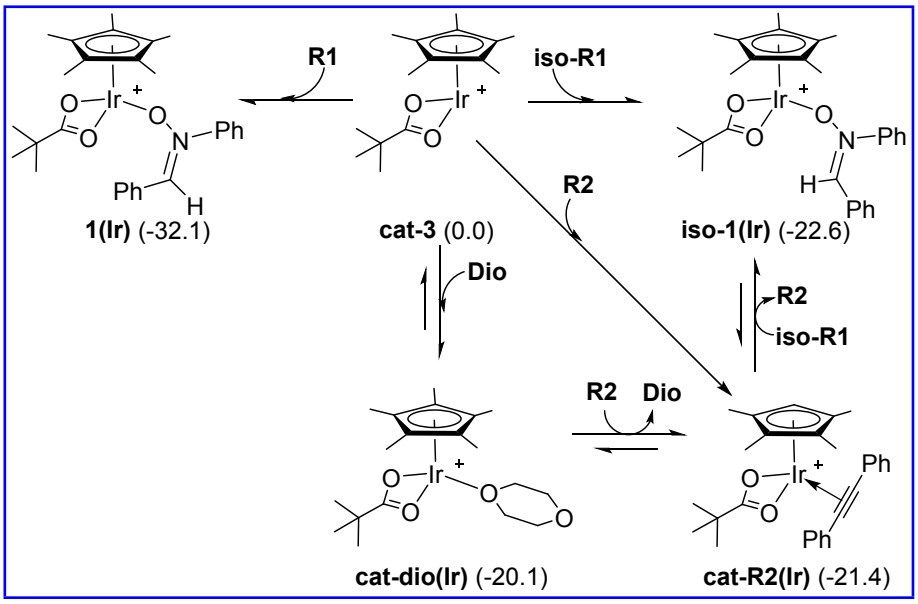


Fig. S2 Comparing the key intermediates and transition states optimized in 1,4-dioxane and the gas phase, respectively. The values in parentheses are the ones in the gas phase. Bond distances are given in Å and relative free energies are given in kcal/mol.



Scheme S1 Possible isomers of the **cat–X** coordination and their relative stabilities. Values in parentheses are relative free energies in kcal/mol, where the energy of **cat-3** is set to be the zero reference energy point.

Cartesian coordinates and Gibbs free energies for all of the calculated structures

cat-1

Sum of electronic and thermal Free Energies: -845.585615

Rh	0.36172	0.00009	-0.1722
C	-1.35365	1.18323	0.54371
C	-1.62955	0.73558	-0.77869
C	-1.62951	-0.73491	-0.77939
C	-1.35358	-1.18389	0.54258
C	-1.13108	-0.00075	1.3662
O	2.16455	-1.09224	-0.1505
C	2.83926	0.00085	-0.19669
O	2.16441	1.09359	-0.15076
C	4.32723	0.00011	-0.27284
C	-0.84677	-0.00142	2.82904
H	-0.2911	0.88633	3.13656
H	-1.8001	-0.00176	3.37568
H	-0.29095	-0.88937	3.13571
C	-1.2855	2.59779	1.02303
H	-1.07393	3.29121	0.20769
H	-2.24699	2.88379	1.46715
H	-0.51492	2.72813	1.78591
C	-1.90653	1.58983	-1.97162
H	-1.5024	1.15178	-2.88718
H	-2.99164	1.68703	-2.10686
H	-1.49331	2.59323	-1.85823
C	-1.90645	-1.58805	-1.9731
H	-1.4914	-2.59091	-1.86154
H	-2.99157	-1.68694	-2.10708
H	-1.50426	-1.14807	-2.88858
C	-1.2855	-2.59897	1.02042
H	-2.24724	-2.88565	1.46354
H	-1.07322	-3.29145	0.20446
H	-0.51544	-2.72998	1.78369
C	4.82082	-1.23983	-1.04128
H	5.86763	-1.14268	-1.24044
H	4.64975	-2.11625	-0.45176
H	4.28804	-1.3221	-1.96555
C	4.88981	-0.07116	1.15895
H	5.95917	-0.0747	1.12222
H	4.55489	0.7785	1.71646
H	4.54624	-0.96678	1.63299
C	4.83102	1.29956	-0.92798
H	5.8916	1.24514	-1.05876
H	4.36013	1.42452	-1.88064
H	4.59137	2.1319	-0.29975

R1

Sum of electronic and thermal Free Energies: -631.750702

C	-4.09565	-0.75994	0.627
C	-2.74213	-1.06363	0.49523
C	-1.88492	-0.12609	-0.08843
C	-2.371	1.08523	-0.58394
C	-3.73073	1.3748	-0.45534
C	-4.59194	0.46242	0.15911
H	-4.76118	-1.47446	1.10183
H	-2.32687	-2.00496	0.83008
H	-1.71025	1.77889	-1.09317
H	-4.11695	2.3097	-0.84763
H	-5.64976	0.69078	0.25811
C	0.44801	0.45078	-0.00392
C	1.88143	0.2521	0.00214
C	2.52591	-0.96416	-0.31867
C	2.67927	1.35984	0.371
C	3.9155	-1.05087	-0.26909
H	1.92112	-1.81416	-0.59799
C	4.06451	1.259	0.42899
H	2.19602	2.30021	0.62238
C	4.69112	0.04965	0.10885
H	4.39793	-1.99148	-0.52265
H	4.65562	2.11656	0.7286
H	5.77199	-0.03541	0.15754
N	-0.47321	-0.4875	-0.16636
O	-0.2332	-1.73558	-0.31149
H	0.06412	1.44678	0.18173

1

Sum of electronic and thermal Free Energies: -1477.362111

Rh	-1.29705	-1.3164	3.19518
C	-1.90835	-1.71695	5.25004

C	-2.64872	-0.56717	4.74715
C	-3.4575	-1.01202	3.64805
C	-3.1915	-2.41128	3.42232
C	-2.25123	-2.84965	4.43936
O	0.41642	-2.42582	2.41838
C	1.22172	-1.53006	2.84512
O	0.7203	-0.57133	3.52785
C	2.71377	-1.57164	2.53977
C	-1.74793	-4.24878	4.59695
H	-0.81892	-4.28474	5.16752
H	-2.49416	-4.85142	5.12942
H	-1.56786	-4.71862	3.62748
C	-0.99094	-1.70061	6.43184
H	-0.38389	-0.79279	6.45132
H	-1.57611	-1.73566	7.35892
H	-0.31451	-2.55684	6.43032
C	-2.63036	0.80511	5.34441
H	-2.83565	1.57529	4.59803
H	-3.39328	0.88486	6.12906
H	-1.66261	1.02683	5.79928
C	-4.42847	-0.1687	2.88426
H	-4.59621	-0.55806	1.87851
H	-5.39516	-0.16539	3.40301
H	-4.0931	0.86803	2.80732
C	-3.8666	-3.30132	2.42575
H	-4.76045	-3.7556	2.87182
H	-4.17811	-2.75294	1.53509
H	-3.20787	-4.11116	2.10552
C	3.09221	-2.90907	1.88303
H	4.16549	-2.92195	1.66969
H	2.86614	-3.75495	2.53866
H	2.55455	-3.06009	0.94356
C	3.49102	-1.37879	3.86038
H	4.56563	-1.35652	3.65465
H	3.21345	-0.44213	4.34959
H	3.30175	-2.20212	4.55748
C	3.01983	-0.39713	1.57915
H	4.08667	-0.39222	1.33552
H	2.45942	-0.49334	0.64352
H	2.76548	0.56246	2.03643
C	0.2161	3.74612	2.19053
C	-0.07835	2.43078	1.83195
C	-1.35463	2.12805	1.34247
C	-2.34273	3.11106	1.23792
C	-2.03073	4.42057	1.60247
C	-0.75545	4.74315	2.07239
H	1.20396	3.98703	2.56988
H	0.67456	1.65902	1.95316
H	-3.33103	2.84027	0.887
H	-2.78912	5.19171	1.51158
H	-0.51981	5.76515	2.35143
C	-2.78687	0.51317	0.24415
C	-3.24284	-0.76296	-0.25054
C	-2.6306	-2.01406	0.00806
C	-4.40769	-0.72399	-1.05534
C	-3.17231	-3.17076	-0.54477
H	-1.76334	-2.06481	0.65101
C	-4.93524	-1.88625	-1.60064
H	-4.89237	0.22917	-1.24959
C	-4.31563	-3.11445	-1.34756
H	-2.70512	-4.12819	-0.33597
H	-5.82776	-1.83976	-2.21606
H	-4.72974	-4.02618	-1.76727
N	-1.70021	0.78202	0.93233
O	-0.93339	-0.19448	1.39724
H	-3.41218	1.37533	0.04523
H	4.64975	-2.11625	-0.45176

Dio

Sum of electronic and thermal Free Energies: -307.559278

C	0.95098	1.15686	0.
C	3.04368	2.36461	0.
C	2.34602	3.57312	-0.0012
C	0.2536	2.36484	-0.00068
H	0.63479	0.60873	-0.86283
H	3.67531	2.36498	0.86368
H	2.6625	4.12009	-0.86466
H	-0.37858	2.36546	0.86259
O	0.9512	3.57304	-0.00168
O	2.34614	1.15686	0.
H	-0.37897	2.36426	-0.86367
H	0.63479	0.6097	0.86344
H	3.67679	2.36412	-0.8626
H	2.66191	4.12146	0.86161

cat-dio

Sum of electronic and thermal Free Energies: -1293.108527

C	2.26419300	-0.33590700	-0.19538100
C	2.97291900	0.75493500	0.23157500

C	4.43655100	-0.90368600	-0.39760900
C	5.65184200	-1.54595500	-0.64749100
C	6.82023700	-0.83996400	-0.37832200
C	6.77843800	0.47312500	0.13009300
C	5.56723400	1.10925700	0.37576300
C	4.36947900	0.42532300	0.10966400
H	5.68575600	-2.55970500	-1.03697700
H	7.78116700	-1.31128600	-0.56215100
H	7.70979000	0.99447600	0.33068400
H	5.54683800	2.12342400	0.76499000
N	3.13721100	-1.35183900	-0.55754600
H	2.87387400	-2.21771500	-0.99944700
N	0.21841500	0.89701900	-0.10493600
C	-1.24098100	0.98971500	-0.19882000
H	-1.56001100	0.25342900	-0.94829800
H	-1.75604400	0.71177000	0.73758300
C	-1.68210800	2.35952200	-0.63408100
H	-1.19435600	2.74617400	-1.52890900
C	-2.62068200	3.09519800	-0.01549400
H	-3.09174300	2.69919600	0.88559300
C	-3.07402100	4.40285000	-0.46320700
H	-2.60184600	4.80078000	-1.36236700
C	2.28161100	2.00083600	0.69602600
H	2.75235200	2.40754200	1.60027000
H	2.34214900	2.78430500	-0.07176800
C	0.80592000	1.68274100	0.98501600
H	0.72631000	1.16650300	1.96076900
H	0.23124300	2.60837000	1.07036000
C	-1.02463600	-2.09896700	0.57620900
C	-2.10369400	-2.61449400	0.33762700
Si	-3.73418200	-3.39428400	-0.00228700
C	-4.89079900	-3.05495300	1.45287800
H	-4.49170700	-3.47334700	2.38248200
H	-5.03327100	-1.98019400	1.60460700
H	-5.87614500	-3.50238600	1.27954800
C	-4.44929000	-2.65241300	-1.58657700
H	-3.78730300	-2.82597600	-2.44115100
H	-5.42190700	-3.09981600	-1.82128300
H	-4.59377900	-1.57148400	-1.49004800
C	-3.49053200	-5.25651200	-0.21391100
H	-2.81719400	-5.47771700	-1.04834700
H	-3.06310600	-5.70578500	0.68828400
H	-4.44652400	-5.75341200	-0.41472300
C	0.76788000	-0.45384000	-0.23729100
H	0.45671700	-0.83671500	-1.21978300
C	0.28543100	-1.51011100	0.83490800
H	1.02773900	-2.31731600	0.88017400
H	0.30387900	-1.03718000	1.82444200
C	-4.01849000	5.13139400	0.15431100
H	-4.48597600	4.72398400	1.05188800
C	-4.49620600	6.48042900	-0.28993800
H	-4.33838900	7.23591300	0.49084300
H	-3.97737700	6.81400600	-1.19353700
H	-5.57374000	6.47274200	-0.50001600

R2

Sum of electronic and thermal Free Energies: -539.313540

C	-2.60674	0.00044	-0.00054
C	-1.39431	0.00058	-0.00058
C	0.03531	0.00034	-0.00028
C	0.75329	1.212	-0.0001
C	0.7526	-1.21171	-0.00011
C	2.14563	1.20738	0.00014
H	0.20616	2.14917	-0.00012
C	2.14496	-1.20787	0.00015
H	0.2049	-2.14855	-0.00012
C	2.84683	-0.00045	0.00026
H	2.68563	2.14982	0.00027
H	2.68441	-2.15062	0.00028
H	3.9328	-0.00075	0.00049
C	-4.14674	-0.00027	0.00049
C	-4.84375	-1.20667	-0.07182
C	-4.84475	1.20511	0.07383
C	-6.23846	-1.20756	-0.07147
H	-4.29316	-2.15676	-0.13041
C	-6.23989	1.20434	0.07519
H	-4.29556	2.15603	0.13101
C	-6.9368	-0.00171	0.00241
H	-6.78793	-2.15839	-0.1291
H	-6.78997	2.15486	0.13344
H	-8.03648	-0.00266	0.00273

cat-R2

Sum of electronic and thermal Free Energies: -1384.905948

Rh	0.02858	0.42626	0.67633
C	1.29421	0.84443	2.46109
C	0.05106	1.58036	2.53767
C	-1.02522	0.60867	2.6177
C	-0.45307	-0.70418	2.53688
C	0.98891	-0.5585	2.43052

O	-1.21337	1.61174	-0.65158
C	-0.18986	2.08313	-1.25454
O	0.94637	1.71375	-0.80787
C	-0.30865	3.03538	-2.43417
C	1.99368	-1.66758	2.4351
H	2.84056	-1.45006	1.78197
H	2.38059	-1.80619	3.452
H	1.55614	-2.61304	2.1128
C	2.665	1.43698	2.40544
H	2.6542	2.44584	1.9889
H	3.07818	1.49672	3.42128
H	3.34306	0.82242	1.80853
C	-0.09033	3.06551	2.66365
H	-1.04399	3.4124	2.26007
H	-0.04568	3.36085	3.71893
H	0.70921	3.59002	2.1372
C	-2.47902	0.92548	2.75557
H	-3.1021	0.16962	2.27323
H	-2.75016	0.9561	3.81841
H	-2.72221	1.8969	2.32123
C	-1.1929	-1.99872	2.65642
H	-1.23288	-2.30155	3.71045
H	-2.21819	-1.9168	2.29169
H	-0.69996	-2.79797	2.10059
C	-1.78727	3.29334	-2.7723
H	-1.85171	3.9773	-3.62448
H	-2.30419	2.36769	-3.04105
H	-2.32024	3.7483	-1.93201
C	0.41905	2.39571	-3.64024
H	0.35999	3.07091	-4.49951
H	1.47253	2.2146	-3.41475
H	-0.04377	1.44577	-3.92669
C	0.39227	4.3597	-2.04434
H	0.36225	5.04983	-2.89311
H	-0.11233	4.84623	-1.20183
H	1.4387	4.19201	-1.77467
C	-0.62666	-1.37628	-0.7815
C	-1.99643	-1.79226	-0.90254
C	-2.2574	-3.18107	-0.93153
C	-3.0679	-0.88385	-1.02937
C	-3.55932	-3.644	-1.09487
H	-1.43702	-3.88301	-0.84262
C	-4.36709	-1.36168	-1.18277
H	-2.86589	0.18129	-1.01995
C	-4.61865	-2.73596	-1.21794
H	-3.7487	-4.71408	-1.12779
H	-5.18578	-0.65645	-1.28322
H	-5.63315	-3.10079	-1.3452
C	0.6124	-1.31311	-0.82355
C	1.9833	-1.64351	-1.11098
C	2.28357	-2.99854	-1.36847
C	3.01647	-0.68738	-1.15264
C	3.58709	-3.38305	-1.66732
H	1.4905	-3.73814	-1.34082
C	4.31764	-1.08673	-1.4513
H	2.78602	0.35682	-0.9732
C	4.60811	-2.42987	-1.70814
H	3.80554	-4.42781	-1.86917
H	5.1087	-0.34296	-1.49287
H	5.62364	-2.73276	-1.94262

iso-R1

Sum of electronic and thermal Free Energies: -631.738491

C	-4.14014	-0.77176	0.48656
C	-2.7842	-1.08343	0.4208
C	-1.88525	-0.12222	-0.0427
C	-2.33026	1.12726	-0.47962
C	-3.69189	1.42568	-0.41407
C	-4.59777	0.48255	0.07394
H	-4.84205	-1.5127	0.8573
H	-2.39929	-2.05317	0.7111
H	-1.63451	1.84695	-0.89686
H	-4.04355	2.39251	-0.76139
H	-5.65659	0.71888	0.12001
C	0.45173	0.41971	0.11922
C	0.75949	1.80775	0.38592
C	-0.20275	2.83065	0.54032
C	2.12702	2.14717	0.50138
C	0.20564	4.13642	0.80422
H	-1.24897	2.57574	0.4488
C	2.52195	3.45337	0.76201
H	2.879	1.37039	0.38446
C	1.56016	4.45692	0.91556
H	-0.54513	4.91284	0.92196
H	3.57845	3.69124	0.84646
H	1.86619	5.47906	1.11912
N	-0.47637	-0.50128	-0.08951
O	-0.24797	-1.74269	-0.30595
H	1.4713	0.06121	0.07935

iso-1

Sum of electronic and thermal Free Energies: -1477.351021

Rh	-0.44959	2.56244	-0.96485
C	-0.88226	4.60082	-0.30488
C	0.42634	4.19822	0.18653
C	1.27588	3.98147	-0.95816
C	0.49384	4.16892	-2.1458
C	-0.84679	4.57012	-1.73708
O	-1.91016	1.38231	-2.11148
C	-2.48404	1.02466	-1.02797
O	-2.05297	1.54005	0.05964
C	-3.61827	0.00757	-1.0063
C	-1.96172	4.91587	-2.67248
H	-2.93464	4.85018	-2.1831
H	-1.8371	5.94201	-3.0396
H	-1.97428	4.24842	-3.53703
C	-2.0443	4.97592	0.55847
H	-2.1189	4.32312	1.43106
H	-1.92065	6.00531	0.9168
H	-2.98866	4.92098	0.01508
C	0.83906	4.15911	1.62489
H	1.68764	3.49033	1.7831
H	1.13646	5.16012	1.96202
H	0.02058	3.8226	2.2653
C	2.73275	3.6485	-0.90139
H	3.07426	3.17114	-1.82047
H	3.31147	4.57086	-0.76767
H	2.96663	2.99258	-0.05924
C	0.97779	4.09043	-3.5597
H	1.32496	5.07647	-3.89367
H	1.80624	3.38823	-3.66658
H	0.18097	3.77417	-4.23613
C	-4.04507	-0.35927	-2.43665
H	-4.86607	-1.08196	-2.39982
H	-4.38934	0.5187	-2.99062
H	-3.22211	-0.80856	-2.99916
C	-4.80571	0.6206	-0.23047
H	-5.61762	-0.11002	-0.16352
H	-4.5104	0.90342	0.78266
H	-5.19694	1.50877	-0.73837
C	-3.10241	-1.24569	-0.25992
H	-3.89522	-1.99899	-0.21747
H	-2.24267	-1.68792	-0.77416
H	-2.80192	-0.99874	0.76122
C	3.10489	-1.07015	2.86741
C	2.93473	-0.79592	1.51138
C	1.87209	0.02332	1.11356
C	0.96466	0.54237	2.03907
C	1.15175	0.26165	3.39327
C	2.2194	-0.53647	3.80987
H	3.92839	-1.70091	3.18681
H	3.62195	-1.20071	0.77693
H	0.12172	1.1288	1.6953
H	0.4584	0.66961	4.12172
H	2.36009	-0.74861	4.86509
C	2.58989	0.37467	-1.21596
C	4.03708	0.45492	-1.10089
C	4.73047	0.96167	0.01922
C	4.77247	0.08958	-2.2486
C	6.11577	1.06916	-0.00985
H	4.1874	1.29536	0.89511
C	6.16049	0.1818	-2.26233
H	4.24634	-0.27002	-3.12865
C	6.83565	0.66994	-1.14165
H	6.63892	1.47495	0.85017
H	6.71291	-0.1135	-3.14844
H	7.91777	0.75488	-1.15349
N	1.66254	0.31179	-0.28825
O	0.41953	0.62423	-0.66066
H	2.1582	0.44681	-2.21009

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Sum of electronic and thermal Free Energies: -1477.332244

Rh	-0.89889	-0.38906	-0.401
C	-1.54717	-0.64878	-2.47495
C	-0.5772	-1.6819	-2.19141
C	-1.08024	-2.49698	-1.1222
C	-2.40539	-2.00046	-0.78292
C	-2.69102	-0.86512	-1.61069
O	-1.34623	1.67378	-0.24054
C	-1.26408	2.34963	0.85368
O	-0.85131	1.87776	1.93599
C	-1.77863	3.80822	0.83382
C	-3.93555	-0.03711	-1.65649
H	-3.67003	1.02627	-1.58984
H	-4.46288	-0.19699	-2.61025
H	-4.62468	-0.2717	-0.84031
C	-1.4607	0.37795	-3.57027
H	-0.42993	0.57033	-3.85385

H	-2.02513	0.03411	-4.4701
H	-1.8953	1.33117	-3.24792
C	0.74317	-1.81812	-2.88314
H	1.24491	-2.74786	-2.61855
H	0.60093	-1.80568	-3.96693
H	1.40591	-0.98989	-2.61915
C	-0.44382	-3.7378	-0.57049
H	-0.59436	-3.82685	0.50701
H	-0.87712	-4.62801	-1.04237
H	0.63094	-3.75385	-0.75912
C	-3.33906	-2.65951	0.18301
H	-3.93804	-3.4052	-0.35298
H	-2.79982	-3.17989	0.974
H	-4.03116	-1.95093	0.64273
C	-1.90038	4.34016	-0.60486
H	-2.20162	5.39044	-0.58751
H	-0.94599	4.27095	-1.13707
H	-2.64413	3.78442	-1.17825
C	-0.82482	4.70502	1.65957
H	-1.19541	5.73331	1.69996
H	-0.71438	4.32305	2.68151
H	0.17558	4.73056	1.20519
C	-3.16615	3.76849	1.52076
H	-3.63021	4.76197	1.45695
H	-3.83868	3.06652	1.0287
H	-3.09488	3.47757	2.57454
C	0.50978	-2.8907	3.38094
C	1.39944	-2.22376	2.54085
C	0.92507	-1.14488	1.7997
C	-0.42404	-0.73798	1.85358
C	-1.28595	-1.43719	2.71472
C	-0.82844	-2.50599	3.4777
H	0.88165	-3.72777	3.97371
H	2.42965	-2.5637	2.46076
H	-0.66302	0.43213	1.72314
H	-2.3162	-1.10528	2.8079
H	-1.50122	-3.03303	4.14604
C	3.07284	-0.30993	1.06477
C	4.05664	0.27418	0.188
C	3.77514	1.01763	-0.98358
C	5.40704	0.05988	0.55606
C	4.82238	1.51463	-1.75026
H	2.74673	1.2085	-1.25916
C	6.44271	0.55286	-0.22276
H	5.6329	-0.5066	1.45389
C	6.15136	1.28287	-1.37854
H	4.60278	2.09294	-2.64293
H	7.47338	0.37439	0.06747
H	6.95875	1.67847	-1.98377
N	1.77651	-0.41821	0.88766
O	1.17038	0.13028	-0.16431
H	3.4245	-0.74506	1.99136

2

Sum of electronic and thermal Free Energies: -1477.354857

C	-0.68064	-0.73951	2.13201
C	-1.09597	-0.9281	3.4545
H	-2.12377	-1.17056	3.70158
C	-0.15878	-0.82803	4.48006
C	1.17565	-0.54933	4.18011
H	1.90492	-0.45853	4.97951
C	1.57969	-0.40513	2.84867
C	0.66868	-0.51051	1.78553
H	0.78744	1.60937	1.74748
H	2.62647	-0.2059	2.64095
C	2.18141	-0.63109	-2.25109
C	3.07896	-0.45125	-1.09927
C	2.97501	-1.60478	-0.26389
C	1.88687	-2.40785	-0.77788
C	1.46993	-1.82575	-2.06263
O	0.52764	1.69309	-0.54553
C	0.44156	2.66165	0.21826
O	0.61472	2.55114	1.52705
C	0.1149	4.07549	-0.2521
Rh	1.03518	-0.50454	-0.22887
H	-0.47306	-0.97283	5.50822
C	1.46142	-3.75184	-0.27079
H	0.3996	-3.92851	-0.45828
H	2.02561	-4.54592	-0.7764
H	1.63631	-3.8499	0.80268
C	0.41141	-2.41889	-2.93944
H	0.76101	-3.36364	-3.37223
H	-0.49419	-2.63535	-2.36433
H	0.14209	-1.7522	-3.76037
C	3.86942	-1.97158	0.87851
H	3.32795	-2.4814	1.67751
H	4.65055	-2.65323	0.51937
H	4.37151	-1.09973	1.30312
C	4.06789	0.66689	-0.9727

H	4.43745	0.77051	0.04959
H	4.93304	0.48545	-1.62292
H	3.62599	1.62007	-1.27351
C	2.05922	0.34899	-3.37656
H	1.28402	0.05454	-4.08584
H	1.80875	1.3458	-3.0007
H	3.00531	0.42644	-3.92486
N	-1.60325	-0.76701	1.02368
O	-1.03841	-0.84689	-0.18281
C	-1.25012	4.47063	0.36585
H	-1.21456	4.4519	1.45798
H	-1.50727	5.48519	0.04803
H	-2.04874	3.80099	0.02906
C	0.0345	4.1129	-1.78587
H	-0.22264	5.12462	-2.11174
H	0.99169	3.84521	-2.24359
H	-0.72679	3.42618	-2.1653
C	1.21587	5.03658	0.25544
H	2.19836	4.76808	-0.14781
H	0.9861	6.0531	-0.07688
H	1.27766	5.03655	1.34604
C	-2.90761	-0.68249	1.14754
H	-3.25007	-0.58787	2.16939
C	-3.9197	-0.68736	0.11979
C	-5.25627	-0.59237	0.57766
C	-3.68258	-0.76981	-1.27273
C	-6.3173	-0.58358	-0.31712
H	-5.45267	-0.5257	1.6438
C	-4.75451	-0.75853	-2.15935
H	-2.66732	-0.83599	-1.63442
C	-6.06832	-0.66671	-1.69132
H	-7.33559	-0.51165	0.05125
H	-4.56481	-0.82251	-3.22586
H	-6.89604	-0.65987	-2.39394

3

Sum of electronic and thermal Free Energies: -1669.732426

C	-0.41341	2.39068	-0.5504
C	-0.48434	3.66415	-1.1324
H	-1.4292	4.11165	-1.42052
C	0.68725	4.38684	-1.33045
C	1.91583	3.84194	-0.94743
H	2.8317	4.40464	-1.1034
C	1.96886	2.57543	-0.36183
C	0.80833	1.82426	-0.1431
H	2.93443	2.16396	-0.08588
C	1.53579	-1.64008	2.23728
C	2.4424	-0.4942	2.09445
C	1.79397	0.65448	2.65894
C	0.44849	0.271	2.97209
C	0.32241	-1.17751	2.76853
Rh	0.67823	0.02685	0.78232
H	0.63812	5.37459	-1.77644
C	-0.60406	1.12648	3.6057
H	-1.5875	0.92071	3.17493
H	-0.66044	0.92336	4.68252
H	-0.39176	2.18951	3.4772
C	-0.90002	-1.96794	3.12438
H	-0.99943	-2.04591	4.21399
H	-1.80818	-1.48812	2.74812
H	-0.86362	-2.98184	2.7222
C	2.42133	1.98431	2.94182
H	1.70643	2.80369	2.84643
H	2.80717	1.9941	3.96884
H	3.26073	2.19072	2.2758
C	3.89531	-0.5952	1.74325
H	4.29756	0.36063	1.40121
H	4.47426	-0.89902	2.6249
H	4.07738	-1.33045	0.95809
C	1.91162	-3.04815	1.8929
H	1.07537	-3.73727	2.02371
H	2.2593	-3.12909	0.85877
H	2.72781	-3.39142	2.53966
N	-1.58248	1.58298	-0.30723
O	-1.36206	0.46779	0.39078
C	1.57187	-0.8952	-1.30286
C	0.42433	-1.32214	-1.09624
C	-0.83577	-1.96882	-1.36848
C	-1.62469	-1.51531	-2.44331
C	-1.27006	-3.07301	-0.61367
C	-2.81941	-2.15952	-2.75412
H	-1.28623	-0.66811	-3.03179
C	-2.46522	-3.71331	-0.9327
H	-0.65864	-3.43335	0.20673
C	-3.24348	-3.2578	-2.00087
H	-3.41833	-1.80709	-3.58907
H	-2.7864	-4.57362	-0.35262
H	-4.17348	-3.75981	-2.2491
C	2.89008	-0.70378	-1.83989

C	3.85476	-1.72393	-1.69954
C	3.2149	0.44811	-2.58286
C	5.11533	-1.58318	-2.27347
H	3.59872	-2.63169	-1.16238
C	4.47924	0.57848	-3.15295
H	2.47154	1.22492	-2.71466
C	5.43291	-0.43032	-2.99645
H	5.84721	-2.37765	-2.16499
H	4.71788	1.46717	-3.72913
H	6.41577	-0.32406	-3.44508
C	-2.79566	1.88827	-0.70533
H	-2.86031	2.81035	-1.26617
C	-4.03376	1.18261	-0.47308
C	-4.1604	-0.06874	0.17292
C	-5.20467	1.82608	-0.94134
C	-5.41948	-0.63411	0.35006
H	-3.27236	-0.58219	0.50927
C	-6.45578	1.25293	-0.75615
H	-5.12341	2.78471	-1.44673
C	-6.56729	0.02031	-0.10486
H	-5.50526	-1.59545	0.84691
H	-7.34366	1.76372	-1.11645
H	-7.545	-0.42835	0.04377

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Sum of electronic and thermal Free Energies: -1669.709769

C	0.48371	1.47753	-1.7751
C	0.69457	2.41563	-2.78834
H	1.64837	2.47353	-3.30343
C	-0.35726	3.2474	-3.17054
C	-1.60615	3.12206	-2.55242
H	-2.42651	3.76654	-2.8545
C	-1.8032	2.17057	-1.55074
C	-0.76679	1.31454	-1.14742
H	-2.76963	2.10191	-1.0607
C	-2.36447	-2.38946	0.24146
C	-3.13477	-1.39944	-0.48344
C	-2.72779	-1.43825	-1.88382
C	-1.62896	-2.31594	-1.98231
C	-1.38298	-2.89793	-0.65116
Rh	-1.02527	-0.69913	-0.47544
H	-0.20499	3.97812	-3.95946
C	-0.8365	-2.66503	-3.20436
H	0.23725	-2.56694	-3.01447
H	-1.02743	-3.70334	-3.50247
H	-1.0894	-2.02241	-4.0497
C	-0.38203	-3.97639	-0.36881
H	-0.78546	-4.95549	-0.65761
H	0.53991	-3.82451	-0.93536
H	-0.12841	-4.02048	0.69192
C	-3.39272	-0.68406	-2.9951
H	-2.76597	-0.63866	-3.88758
H	-4.33519	-1.17289	-3.27386
H	-3.63154	0.34198	-2.70506
C	-4.33389	-0.67397	0.04608
H	-4.50606	0.26542	-0.48561
H	-5.23367	-1.2888	-0.0812
H	-4.23537	-0.45261	1.11012
C	-2.59486	-2.81747	1.65801
H	-1.67686	-3.16586	2.13422
H	-2.99992	-2.00702	2.26842
H	-3.31817	-3.64221	1.68036
N	1.51842	0.56556	-1.36802
O	1.09691	-0.64461	-1.01616
C	-0.57829	1.22299	0.89936
C	-0.35641	0.03653	1.33679
C	0.01112	-0.66214	2.56046
C	0.9593	-1.70119	2.53479
C	-0.57909	-0.29909	3.78592
C	1.3158	-2.35541	3.71397
H	1.42313	-1.96718	1.58958
C	-0.22607	-0.96632	4.95879
H	-1.30825	0.50564	3.8103
C	0.72047	-1.9943	4.92667
H	2.05907	-3.14772	3.68808
H	-0.68858	-0.68047	5.89944
H	0.99424	-2.50988	5.84275
C	-0.56788	2.6282	1.29294
C	0.6797	3.25322	1.48005
C	-1.7463	3.34806	1.56314
C	0.74394	4.57019	1.93944
H	1.59256	2.6941	1.28286
C	-1.67468	4.66998	2.0091
H	-2.71532	2.86833	1.43465
C	-0.43103	5.28274	2.19753
H	1.71376	5.03896	2.09511
H	-2.59204	5.21939	2.21928
H	-0.37675	6.30883	2.54772
C	2.78596	0.91043	-1.34423

H	2.95883	1.94819	-1.59981
C	3.94015	0.09873	-1.04165
C	3.91369	-1.28382	-0.74834
C	5.18729	0.76695	-1.06255
C	5.10248	-1.9595	-0.48829
H	2.96646	-1.80313	-0.73816
C	6.36647	0.08283	-0.79733
H	5.22053	1.82917	-1.29111
C	6.32669	-1.28496	-0.50921
H	5.07626	-3.02246	-0.26875
H	7.31486	0.61017	-0.81787
H	7.2476	-1.82282	-0.30413

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Sum of electronic and thermal Free Energies: -1669.750234

C	0.8691	-0.04406	-2.2509
C	1.03133	-0.54824	-3.54413
H	1.73402	-1.35713	-3.71792
C	0.28272	-0.01189	-4.58825
C	-0.62093	1.0225	-4.32558
H	-1.20273	1.45276	-5.13479
C	-0.76647	1.519	-3.03279
C	-0.0343	0.9961	-1.9482
H	-1.43649	2.35187	-2.84472
C	-2.82309	-1.42944	1.26315
C	-3.32096	-1.30096	-0.06336
C	-2.76994	-2.408	-0.87617
C	-1.87511	-3.13422	-0.08722
C	-1.80351	-2.46466	1.22105
Rh	-1.13806	-0.91368	-0.10184
H	0.40542	-0.39597	-5.5955
C	-1.02891	-4.30654	-0.47721
H	0.03535	-4.07715	-0.35732
H	-1.2557	-5.17512	0.15138
H	-1.19454	-4.59528	-1.51671
C	-1.02184	-2.96323	2.39366
H	-1.6002	-3.72969	2.92732
H	-0.08132	-3.42111	2.07892
H	-0.79931	-2.15966	3.09918
C	-3.12258	-2.63048	-2.31369
H	-2.48394	-3.38303	-2.77895
H	-4.16276	-2.96632	-2.40473
H	-3.03231	-1.70513	-2.89215
C	-4.39778	-0.36902	-0.52918
H	-4.23208	-0.04782	-1.56083
H	-5.37489	-0.86768	-0.49452
H	-4.45534	0.52317	0.09749
C	-3.31017	-0.7432	2.49738
H	-2.49205	-0.43214	3.14956
H	-3.9066	0.13981	2.26318
H	-3.94846	-1.43359	3.06353
N	1.6335	-0.66248	-1.18569
O	0.93178	-1.40751	-0.3381
C	-0.13054	1.64629	-0.58907
C	-0.49966	0.92508	0.49642
C	-0.42841	1.37068	1.90061
C	0.76872	1.15124	2.61079
C	-1.4928	1.99706	2.57234
C	0.8986	1.5597	3.93697
H	1.60025	0.66682	2.10777
C	-1.36017	2.4068	3.89994
H	-2.42502	2.17704	2.0458
C	-0.16486	2.19013	4.58751
H	1.83557	1.39371	4.46081
H	-2.19029	2.90245	4.39487
H	-0.06094	2.51356	5.61867
C	0.1275	3.1225	-0.59489
C	-0.81042	4.02632	-0.07123
C	1.29523	3.639	-1.18307
C	-0.58089	5.40162	-0.11559
H	-1.73249	3.64954	0.356
C	1.52872	5.01269	-1.22052
H	2.02825	2.95954	-1.61036
C	0.59016	5.89941	-0.68739
H	-1.32347	6.08343	0.2892
H	2.4412	5.39264	-1.67038
H	0.76699	6.97006	-0.72546
C	2.93844	-0.56137	-1.13223
H	3.35846	0.05272	-1.92142
C	3.85086	-1.17666	-0.1951
C	3.46645	-1.96166	0.91615
C	5.22767	-0.9638	-0.43775
C	4.43948	-2.5094	1.74616
H	2.41619	-2.12567	1.10923
C	6.18973	-1.52334	0.39312
H	5.53492	-0.36037	-1.28755
C	5.79691	-2.29879	1.48832
H	4.13814	-3.10996	2.59899
H	7.24288	-1.35825	0.19043

H	6.54738	-2.73805	2.13843

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Sum of electronic and thermal Free Energies: -1669.701890

C	-0.77985	-0.28883	2.15006
C	-1.2741	0.0559	3.41583
H	-2.32517	0.28138	3.56944
C	-0.38395	0.14599	4.47895
C	0.97728	-0.08631	4.25557
H	1.67958	-0.00492	5.08025
C	1.44505	-0.39389	2.97614
C	0.58527	-0.51029	1.87272
H	2.51256	-0.53096	2.83481
C	2.77342	-1.3788	-1.58413
C	3.12107	-1.66054	-0.18998
C	2.34938	-2.82809	0.23431
C	1.43342	-3.11758	-0.79494
C	1.70048	-2.21936	-1.928
Rh	1.10008	-0.91821	-0.06527
H	-0.74449	0.41658	5.46557
C	0.41093	-4.21377	-0.81598
H	-0.52135	-3.88597	-1.28546
H	0.778	-5.07009	-1.3958
H	0.17704	-4.57115	0.189
C	0.99242	-2.29323	-3.24795
H	1.37516	-3.13113	-3.84426
H	-0.08213	-2.45498	-3.12134
H	1.12998	-1.38154	-3.83277
C	2.54364	-3.57542	1.51835
H	1.6843	-4.20663	1.75394
H	3.42425	-4.22584	1.4472
H	2.70166	-2.90147	2.36377
C	4.33601	-1.12782	0.50655
H	4.27205	-1.25572	1.58968
H	5.22977	-1.66927	0.1691
H	4.49168	-0.06798	0.29376
C	3.47651	-0.38518	-2.45616
H	2.87505	-0.10776	-3.32428
H	3.72036	0.52993	-1.91199
H	4.41736	-0.81235	-2.82568
N	-1.69456	-0.439	1.04624
O	-1.14153	-0.22441	-0.20405
C	0.83641	1.11225	-0.32481
C	-0.47011	1.32162	-0.32678
C	-1.47686	2.36747	-0.26482
C	-1.25284	3.46402	0.59208
C	-2.6434	2.34292	-1.05179
C	-2.16682	4.51372	0.6442
H	-0.35667	3.48587	1.20318
C	-3.56283	3.38588	-0.97847
H	-2.82106	1.50942	-1.72226
C	-3.32536	4.47499	-0.13506
H	-1.97992	5.35712	1.30173
H	-4.45988	3.35716	-1.58952
H	-4.04052	5.29048	-0.08689
C	1.83809	2.16883	-0.54724
C	2.88415	2.36297	0.37418
C	1.77673	2.9981	-1.68246
C	3.82938	3.3681	0.17252
H	2.93553	1.73452	1.25747
C	2.73362	3.99178	-1.88693
H	0.97778	2.85502	-2.40357
C	3.76112	4.18253	-0.96072
H	4.62187	3.51492	0.90062
H	2.67404	4.61992	-2.77083
H	4.50328	4.95852	-1.12075
C	-2.93129	-0.85284	1.12844
H	-3.234	-1.05499	2.15044
C	-3.9149	-1.10816	0.10535
C	-3.67635	-1.14101	-1.2895
C	-5.21633	-1.39499	0.58276
C	-4.71704	-1.43654	-2.16135
H	-2.68256	-0.95187	-1.66913
C	-6.25132	-1.67658	-0.29933
H	-5.40866	-1.38693	1.65203
C	-6.00319	-1.69722	-1.67442
H	-4.52729	-1.46697	-3.22954
H	-7.24568	-1.88513	0.08121
H	-6.80834	-1.92326	-2.36668

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Sum of electronic and thermal Free Energies: -1669.710049

C	-0.80382	-0.26523	2.14026
C	-1.30405	0.09544	3.39914
H	-2.35306	0.34193	3.53498
C	-0.42307	0.16887	4.47086
C	0.93425	-0.09301	4.25768
H	1.63189	-0.02404	5.08746
C	1.40697	-0.41405	2.98299
C	0.55854	-0.51729	1.86858

H	2.47297	-0.57196	2.85458
C	2.82271	-1.33063	-1.55621
C	3.14912	-1.61656	-0.15655
C	2.415	-2.82249	0.23839
C	1.53131	-3.12764	-0.80883
C	1.78363	-2.1998	-1.92526
Rh	1.11541	-0.93382	-0.06377
H	-0.78575	0.44977	5.45374
C	0.54072	-4.25122	-0.86393
H	-0.40333	-3.93316	-1.31688
H	0.92764	-5.07537	-1.47646
H	0.32292	-4.65048	0.1287
C	1.0971	-2.27851	-3.25596
H	1.52102	-3.09025	-3.86067
H	0.02826	-2.48517	-3.14757
H	1.20632	-1.35179	-3.82276
C	2.61371	-3.57468	1.51875
H	1.78682	-4.25915	1.71888
H	3.53369	-4.17026	1.46969
H	2.70336	-2.90384	2.37679
C	4.32936	-1.04833	0.56931
H	4.25579	-1.20004	1.64857
H	5.24864	-1.54702	0.23414
H	4.44343	0.02049	0.37686
C	3.51368	-0.30932	-2.40518
H	2.92152	-0.04184	-3.28272
H	3.71968	0.60766	-1.84875
H	4.47337	-0.70628	-2.7598
N	-1.72635	-0.40836	1.04458
O	-1.18947	-0.12003	-0.22761
C	0.77277	1.08022	-0.31021
C	-0.55889	1.22859	-0.29247
C	-1.49343	2.36051	-0.25004
C	-1.14719	3.51466	0.47881
C	-2.72973	2.33196	-0.91992
C	-2.00858	4.6079	0.52421
H	-0.20031	3.5465	1.00677
C	-3.5941	3.42372	-0.86055
H	-3.00936	1.45964	-1.50025
C	-3.23624	4.56582	-0.14135
H	-1.72541	5.49074	1.0893
H	-4.54372	3.387	-1.38614
H	-3.90855	5.41733	-0.10032
C	1.74397	2.15843	-0.53829
C	2.77869	2.39896	0.38611
C	1.67627	2.96009	-1.69371
C	3.70264	3.42092	0.16957
H	2.83786	1.7929	1.28477
C	2.61199	3.97027	-1.91333
H	0.8861	2.78382	-2.41715
C	3.62655	4.20684	-0.98308
H	4.48434	3.6033	0.90134
H	2.54608	4.57616	-2.81222
H	4.35187	4.99613	-1.15485
C	-2.9297	-0.90843	1.11125
H	-3.20336	-1.17765	2.12687
C	-3.91168	-1.17568	0.09025
C	-3.68712	-1.15696	-1.3074
C	-5.19337	-1.53491	0.57277
C	-4.72468	-1.46858	-2.17708
H	-2.7068	-0.91761	-1.69399
C	-6.22603	-1.83119	-0.307
H	-5.37283	-1.56869	1.64372
C	-5.99317	-1.79726	-1.68457
H	-4.54626	-1.45846	-3.2475
H	-7.20626	-2.09345	0.07681
H	-6.79635	-2.03478	-2.37526

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Sum of electronic and thermal Free Energies: -1669.720820

C	-0.62636	-0.4845	2.35649
C	-0.77168	-1.19185	3.5593
H	-1.70993	-1.69927	3.76107
C	0.28202	-1.26315	4.45638
C	1.4943	-0.632	4.13271
H	2.33192	-0.68676	4.82132
C	1.64392	0.05346	2.93887
C	0.59128	0.15801	1.98869
H	2.58799	0.53566	2.71456
C	1.82437	-1.70917	-2.35586
C	2.8066	-1.50914	-1.30734
C	2.59013	-2.51379	-0.26965
C	1.40119	-3.19076	-0.58782
C	0.90391	-2.68275	-1.87632
Rh	0.87501	-0.93857	-0.44031
H	0.17381	-1.81402	5.38418
C	0.73967	-4.28936	0.18967
H	-0.3463	-4.16226	0.22085
H	0.93844	-5.26194	-0.27743

H	1.10247	-4.33502	1.21832
C	-0.27261	-3.25033	-2.61089
H	0.00592	-4.18368	-3.1174
H	-1.09547	-3.48262	-1.93033
H	-0.6484	-2.56161	-3.37092
C	3.47712	-2.71507	0.92114
H	3.01086	-3.35992	1.66863
H	4.42355	-3.18309	0.62333
H	3.72259	-1.76607	1.40827
C	4.03429	-0.65495	-1.41018
H	4.31587	-0.23309	-0.44217
H	4.8806	-1.25739	-1.76509
H	3.90034	0.16825	-2.11528
C	1.85652	-1.07929	-3.71625
H	0.88597	-1.13624	-4.21424
H	2.15648	-0.02923	-3.67662
H	2.5795	-1.60173	-4.35575
N	-1.70895	-0.41593	1.46709
O	-1.29654	-0.54702	0.05177
C	0.76551	1.01755	0.79507
C	0.07991	0.86167	-0.43332
C	-0.50862	1.81814	-1.3432
C	-0.95945	3.07475	-0.88116
C	-0.69974	1.48321	-2.69866
C	-1.56112	3.97079	-1.75666
H	-0.81929	3.34054	0.16109
C	-1.30505	2.38164	-3.57083
H	-0.37072	0.51028	-3.04536
C	-1.73366	3.6274	-3.10204
H	-1.89796	4.93721	-1.39486
H	-1.4447	2.11657	-4.61429
H	-2.20437	4.32977	-3.78338
C	1.68242	2.19946	0.90998
C	1.61291	3.04015	2.03689
C	2.57102	2.53883	-0.12286
C	2.40803	4.18126	2.12323
H	0.92834	2.80116	2.84494
C	3.36736	3.68043	-0.03421
H	2.63506	1.90301	-0.99888
C	3.28959	4.50516	1.08884
H	2.33657	4.82002	2.99844
H	4.05133	3.92326	-0.84191
H	3.91084	5.39262	1.15937
C	-2.95621	-0.17171	1.77938
H	-3.09064	0.09856	2.82352
C	-4.14386	-0.23956	0.96441
C	-4.17475	-0.55605	-0.41352
C	-5.36218	0.02851	1.63284
C	-5.39309	-0.61496	-1.08035
H	-3.2458	-0.74142	-0.9337
C	-6.57202	-0.0285	0.95409
H	-5.34945	0.27556	2.69106
C	-6.59011	-0.35238	-0.40588
H	-5.41203	-0.86115	-2.13746
H	-7.4986	0.1769	1.4802
H	-7.53454	-0.39625	-0.93964

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Sum of electronic and thermal Free Energies: -1669.726577

C	-0.93048	0.07487	2.52159
C	-1.23252	-0.27736	3.84926
H	-2.20057	-0.70765	4.08719
C	-0.26891	-0.10283	4.82593
C	0.9901	0.42099	4.47117
H	1.74202	0.57183	5.23947
C	1.28829	0.74098	3.15796
C	0.33958	0.56303	2.12142
H	2.25826	1.15448	2.9092
C	2.80021	-1.13146	-1.45728
C	3.30584	-1.72774	-0.21878
C	2.4891	-2.83725	0.06432
C	1.54184	-3.02008	-1.04292
C	1.7741	-2.01256	-2.00711
Rh	1.11422	-0.97012	-0.0921
H	-0.47841	-0.38138	5.85298
C	0.57073	-4.15754	-1.13785
H	-0.20992	-3.96567	-1.87705
H	1.08756	-5.07987	-1.43345
H	0.08714	-4.35669	-0.17688
C	1.13304	-1.8648	-3.3539
H	1.80725	-2.21863	-4.14417
H	0.21056	-2.44528	-3.42408
H	0.88656	-0.82217	-3.57279
C	2.60334	-3.75699	1.24302
H	1.62179	-4.07322	1.60768
H	3.15391	-4.66663	0.97043
H	3.13505	-3.28581	2.07257
C	4.51008	-1.27619	0.55187
H	4.37997	-1.40663	1.6295

H	5.39292	-1.85823	0.25656
H	4.74482	-0.22615	0.36383
C	3.47234	-0.03184	-2.22046
H	2.80722	0.39812	-2.97123
H	3.81922	0.7736	-1.56974
H	4.34846	-0.43206	-2.74802
N	-1.9022	-0.03102	1.51924
O	-1.34926	-0.45648	0.26305
C	0.57536	0.97556	0.72496
C	-0.3511	0.49146	-0.28384
C	-0.77471	1.14452	-1.54701
C	-2.10429	1.09379	-1.99474
C	0.17122	1.80394	-2.35699
C	-2.47675	1.68328	-3.20371
H	-2.85464	0.59199	-1.40012
C	-0.20636	2.3956	-3.55939
H	1.20407	1.85858	-2.03832
C	-1.53291	2.33716	-3.99373
H	-3.51265	1.6285	-3.5253
H	0.54245	2.90121	-4.16203
H	-1.82351	2.7933	-4.93479
C	1.32523	2.26847	0.55148
C	2.72511	2.32739	0.55205
C	0.60619	3.47262	0.47018
C	3.39198	3.5522	0.46656
H	3.29093	1.40506	0.62469
C	1.2697	4.69521	0.3765
H	-0.47973	3.44904	0.4724
C	2.66576	4.73951	0.37389
H	4.47786	3.57606	0.47114
H	0.69565	5.61447	0.30813
H	3.18184	5.69192	0.30229
C	-3.19368	0.17278	1.64578
H	-3.44447	0.71079	2.55733
C	-4.28527	-0.2441	0.8075
C	-4.19135	-1.21075	-0.22307
C	-5.54699	0.32594	1.10282
C	-5.32913	-1.57827	-0.92893
H	-3.2363	-1.66591	-0.45174
C	-6.67393	-0.03713	0.3774
H	-5.62988	1.05752	1.90191
C	-6.56708	-0.99019	-0.63984
H	-5.25545	-2.32698	-1.71098
H	-7.63396	0.41365	0.60608
H	-7.44821	-1.28018	-1.2038

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Sum of electronic and thermal Free Energies: -1669.717490

C	-0.90106	-1.42113	0.81369
C	-1.0912	-2.85095	0.94165
H	-1.777	-3.33983	0.25578
C	-0.46556	-3.56122	1.92659
C	0.38585	-2.90547	2.86898
H	0.8144	-3.47897	3.6849
C	0.6746	-1.57339	2.74919
C	0.10123	-0.78368	1.69582
H	1.33209	-1.08208	3.45783
C	2.60986	-0.47526	-1.88084
C	2.87132	-1.62908	-1.1121
C	1.77561	-2.56046	-1.33039
C	0.89402	-2.0128	-2.34034
C	1.3733	-0.7093	-2.64235
Rh	0.8004	-0.76154	-0.43319
H	-0.63058	-4.63094	2.00973
C	-0.25187	-2.72723	-2.99658
H	-1.00416	-2.02774	-3.36848
H	0.10074	-3.31737	-3.85164
H	-0.74839	-3.41824	-2.31002
C	0.82219	0.23418	-3.66261
H	1.42492	0.17927	-4.57984
H	-0.20915	-0.00994	-3.92832
H	0.84795	1.27046	-3.3147
C	1.7366	-3.95333	-0.78547
H	0.76402	-4.42395	-0.93326
H	2.48669	-4.57032	-1.29624
H	1.9644	-3.97705	0.28376
C	4.08643	-1.91092	-0.28128
H	3.83845	-2.44292	0.64234
H	4.78804	-2.54487	-0.83896
H	4.61839	-0.99424	-0.01718
C	3.51743	0.70353	-2.05803
H	2.96312	1.60492	-2.32262
H	4.09113	0.91431	-1.15168
H	4.23462	0.50597	-2.86518
N	-2.10047	-0.68883	0.47666
O	-1.64963	0.98234	0.56242
C	0.54816	0.5365	1.31493
C	-0.35486	1.16346	0.33367
C	-0.03905	2.23675	-0.65408

C	-1.03208	2.64159	-1.56656
C	1.19561	2.91088	-0.67952
C	-0.80256	3.68	-2.46614
H	-1.98611	2.127	-1.57475
C	1.41377	3.96335	-1.56978
H	1.98326	2.62517	-0.00322
C	0.4206	4.35563	-2.4683
H	-1.58752	3.96398	-3.1707
H	2.36834	4.47921	-1.55759
H	0.59405	5.1753	-3.15975
C	1.59758	1.26747	2.0787
C	2.89472	0.75901	2.25499
C	1.26142	2.48817	2.68936
C	3.83298	1.45445	3.01842
H	3.16675	-0.1793	1.78336
C	2.19961	3.17992	3.45419
H	0.26018	2.89004	2.56475
C	3.48826	2.66672	3.61955
H	4.83361	1.05038	3.14237
H	1.92302	4.11987	3.92188
H	4.21888	3.20779	4.21303
C	-3.31712	-1.045	0.75155
H	-3.44055	-2.01711	1.23333
C	-4.53801	-0.30598	0.50796
C	-4.5927	0.96882	-0.09704
C	-5.74014	-0.92527	0.91802
C	-5.81981	1.59173	-0.2879
H	-3.67525	1.46	-0.38981
C	-6.963	-0.29247	0.72724
H	-5.70586	-1.90717	1.38538
C	-7.00441	0.96784	0.12271
H	-5.85809	2.57008	-0.75517
H	-7.88039	-0.77698	1.04706
H	-7.95805	1.46535	-0.0265

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Sum of electronic and thermal Free Energies: -1669.808976

C	-1.00982	-1.31204	1.72003
C	-1.00642	-2.45981	2.5534
H	-1.89288	-3.08499	2.5541
C	0.06754	-2.76954	3.3673
C	1.20586	-1.94276	3.37467
H	2.0377	-2.15847	4.03716
C	1.25467	-0.85292	2.53229
C	0.19607	-0.5143	1.6275
H	2.12517	-0.20722	2.54589
C	2.86847	-0.57331	-1.99829
C	3.42448	-1.09198	-0.77706
C	2.77557	-2.34905	-0.50998
C	1.85536	-2.64531	-1.5915
C	1.89773	-1.54244	-2.49662
Rh	1.19105	-0.78176	-0.54519
H	0.01672	-3.63627	4.0194
C	1.04595	-3.89509	-1.75279
H	0.06158	-3.68769	-2.20297
H	1.56918	-4.60707	-2.41689
H	0.88187	-4.39286	-0.79285
C	1.11995	-1.4296	-3.77122
H	1.58722	-2.04613	-4.54916
H	0.09335	-1.77971	-3.64138
H	1.08382	-0.40121	-4.13602
C	3.08704	-3.27936	0.61865
H	2.17824	-3.67755	1.08202
H	3.66404	-4.13311	0.23757
H	3.6785	-2.79167	1.39611
C	4.56613	-0.52031	0.00812
H	4.40467	-0.60743	1.08567
H	5.49371	-1.05555	-0.23158
H	4.73199	0.53439	-0.22287
C	3.29109	0.66764	-2.72196
H	2.43785	1.19015	-3.16342
H	3.81755	1.36389	-2.06808
H	3.97063	0.40147	-3.54
N	-2.13862	-1.01728	1.00326
O	-0.75573	-0.09947	-0.999
C	0.37009	0.75795	0.85271
C	-0.34962	0.96878	-0.38714
C	-0.64999	2.27826	-1.02818
C	-1.93066	2.39346	-1.60454
C	0.23066	3.37172	-1.0983
C	-2.33008	3.58363	-2.20671
H	-2.61434	1.55287	-1.55207
C	-0.16547	4.54995	-1.72981
H	1.22537	3.30552	-0.67429
C	-1.44715	4.66411	-2.27575
H	-3.33045	3.6672	-2.62304
H	0.52974	5.38282	-1.79009
H	-1.7554	5.58969	-2.75223
C	1.03679	1.8949	1.57002

C	2.36329	2.27549	1.32255
C	0.31008	2.58806	2.54942
C	2.9492	3.3294	2.02663
H	2.93328	1.74054	0.56515
C	0.89054	3.6449	3.24927
H	-0.71238	2.29952	2.75677
C	2.21519	4.01493	2.99191
H	3.97578	3.61284	1.82209
H	0.30827	4.18116	3.9969
H	2.66785	4.83505	3.54018
C	-3.32192	-0.99843	1.49939
H	-3.48437	-1.05646	2.58634
C	-4.52011	-0.89763	0.66926
C	-4.4313	-0.8501	-0.73628
C	-5.78294	-0.88013	1.28426
C	-5.58845	-0.78385	-1.50288
H	-3.44902	-0.87093	-1.19776
C	-6.94067	-0.81876	0.51076
H	-5.85396	-0.91988	2.36864
C	-6.84416	-0.77026	-0.8817
H	-5.52008	-0.7494	-2.5864
H	-7.91432	-0.81067	0.99063
H	-7.74558	-0.72416	-1.48539

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Sum of electronic and thermal Free Energies: -1669.695232

C	-1.38737	-0.82293	1.96448
C	-1.51406	-1.70804	3.05245
H	-2.06436	-2.63394	2.91764
C	-0.93516	-1.39661	4.27828
C	-0.20248	-0.2137	4.42534
H	0.24829	0.03247	5.38182
C	-0.04172	0.64757	3.33881
C	-0.60794	0.35311	2.0916
H	0.53318	1.56187	3.45598
C	3.48387	-0.34533	-0.86147
C	3.38742	-0.02968	0.51377
C	2.96979	-1.22489	1.20766
C	2.93897	-2.32899	0.2468
C	3.21229	-1.78108	-1.02955
Rh	1.27428	-0.83338	-0.1964
H	-1.0556	-2.07223	5.1195
C	2.68735	-3.76465	0.59049
H	2.34033	-4.33238	-0.27466
H	3.61199	-4.23246	0.95129
H	1.93776	-3.86314	1.37887
C	3.32034	-2.52007	-2.3262
H	4.37317	-2.74329	-2.54189
H	2.7774	-3.46657	-2.30083
H	2.93681	-1.92735	-3.16008
C	2.85062	-1.39276	2.68639
H	2.06209	-2.10009	2.9514
H	3.79755	-1.78571	3.0811
H	2.64278	-0.44821	3.1883
C	3.69673	1.28813	1.15593
H	3.07759	1.46072	2.03862
H	4.7456	1.31259	1.47578
H	3.54041	2.11842	0.46537
C	3.95202	0.55401	-1.96054
H	3.43556	0.35045	-2.90059
H	3.8054	1.60688	-1.71799
H	5.02455	0.39275	-2.13144
N	-1.95862	-1.09487	0.72803
O	-0.17721	-1.82318	-0.41886
C	-0.49735	1.29431	0.92767
C	0.40277	1.02219	-0.05918
C	0.78426	1.91204	-1.16577
C	0.63299	1.50677	-2.50971
C	1.32577	3.19012	-0.90888
C	0.99863	2.3532	-3.55486
H	0.19712	0.5347	-2.72225
C	1.70444	4.02627	-1.95676
H	1.42625	3.5254	0.1186
C	1.54308	3.6114	-3.28275
H	0.85492	2.03414	-4.58296
H	2.11488	5.0082	-1.74088
H	1.83066	4.26867	-4.09753
C	-1.4619	2.43345	0.8991
C	-1.99035	2.91848	-0.31474
C	-1.92195	3.01848	2.09632
C	-2.91008	3.96328	-0.32992
H	-1.6995	2.45778	-1.25019
C	-2.82622	4.078	2.0765
H	-1.56868	2.65054	3.05218
C	-3.3247	4.55706	0.86401
H	-3.31008	4.30902	-1.27834
H	-3.14877	4.52298	3.01298
H	-4.03889	5.37465	0.85028
C	-3.17977	-1.45166	0.55756

H	-3.86677	-1.40918	1.41397
C	-3.77128	-1.88509	-0.70116
C	-3.01137	-2.06566	-1.87358
C	-5.15639	-2.13268	-0.72589
C	-3.63818	-2.47917	-3.04337
H	-1.94174	-1.89082	-1.83829
C	-5.7772	-2.5455	-1.90137
H	-5.74258	-1.99607	0.17931
C	-5.0179	-2.71815	-3.06092
H	-3.05441	-2.62225	-3.94769
H	-6.84615	-2.73255	-1.915
H	-5.49921	-3.042	-3.97893

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Sum of electronic and thermal Free Energies: -1669.703259

C	-1.52515	-1.16663	1.80115
C	-1.77286	-2.13304	2.792
H	-2.47664	-2.93203	2.57883
C	-1.12221	-2.07596	4.02388
C	-0.20646	-1.05587	4.28831
H	0.28423	-0.99409	5.25465
C	0.07422	-0.10919	3.2981
C	-0.55374	-0.16467	2.04855
H	0.76748	0.70081	3.50624
C	3.61016	-0.34365	-0.50679
C	3.26069	-0.61415	0.85185
C	2.68883	-1.92036	0.9078
C	2.7428	-2.50655	-0.43216
C	3.3156	-1.53337	-1.3073
Rh	1.33821	-0.76473	-0.62184
H	-1.33871	-2.82425	4.78046
C	2.36354	-3.91253	-0.77831
H	2.1158	-4.01333	-1.83611
H	3.20156	-4.58723	-0.56034
H	1.505	-4.2535	-0.19606
C	3.67437	-1.72345	-2.74748
H	4.708	-2.08483	-2.82323
H	3.02569	-2.45509	-3.23205
H	3.6108	-0.7881	-3.30704
C	2.26345	-2.66877	2.12597
H	1.41899	-3.33008	1.92036
H	3.09729	-3.29549	2.47042
H	1.97904	-2.00412	2.94015
C	3.53178	0.29665	2.01065
H	2.96013	0.00856	2.89286
H	4.59516	0.25393	2.27462
H	3.29574	1.33653	1.77311
C	4.33562	0.86209	-1.00798
H	4.06849	1.09981	-2.03923
H	4.13828	1.74183	-0.3942
H	5.41661	0.66902	-0.98126
N	-2.14488	-1.17954	0.55082
O	0.18516	-1.24958	-1.8376
C	-0.36694	0.94543	1.05477
C	0.64329	1.00252	0.13957
C	1.1582	2.17457	-0.55896
C	1.23009	2.22627	-1.97101
C	1.6054	3.29414	0.18169
C	1.71588	3.36206	-2.61297
H	0.86501	1.38362	-2.55006
C	2.10276	4.41934	-0.46668
H	1.53533	3.27384	1.26474
C	2.16063	4.45633	-1.86473
H	1.74158	3.39896	-3.69771
H	2.43504	5.27441	0.11387
H	2.54195	5.33933	-2.368
C	-1.42456	1.99693	1.08271
C	-1.90296	2.59155	-0.10125
C	-1.99723	2.38539	2.31061
C	-2.9007	3.56041	-0.05511
H	-1.51653	2.26576	-1.05938
C	-2.97396	3.37714	2.35301
H	-1.66381	1.92332	3.23306
C	-3.4318	3.96557	1.17186
H	-3.27206	3.99259	-0.97926
H	-3.38505	3.68301	3.31011
H	-4.20674	4.72518	1.20607
C	-3.41373	-1.34502	0.44676
H	-4.05446	-1.42017	1.33833
C	-4.0998	-1.40535	-0.8436
C	-3.38282	-1.40694	-2.05556
C	-5.50342	-1.44714	-0.86919
C	-4.06839	-1.44488	-3.26446
H	-2.29752	-1.38276	-2.0246
C	-6.18557	-1.48074	-2.08396
H	-6.05747	-1.44649	0.06637
C	-5.46847	-1.47922	-3.28197
H	-3.51556	-1.45022	-4.19931
H	-7.27057	-1.50812	-2.09714

H	-5.99797	-1.50761	-4.22991

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Sum of electronic and thermal Free Energies: -1669.689583

C	-1.66022	-0.13402	1.989
C	-2.12259	-0.649	3.21406
H	-2.99794	-1.29153	3.21492
C	-1.4609	-0.36719	4.40823
C	-0.30965	0.42248	4.40275
H	0.20604	0.65241	5.32971
C	0.17232	0.92449	3.19034
C	-0.4819	0.6518	1.98225
H	1.0497	1.56482	3.18304
C	3.35466	-1.9494	0.20981
C	2.97838	-1.61188	1.55598
C	1.85518	-2.40441	1.90608
C	1.55897	-3.30881	0.79016
C	2.502	-3.04775	-0.24679
Rh	1.21614	-1.23931	-0.06734
H	-1.84297	-0.76869	5.34207
C	0.52287	-4.38783	0.80742
H	0.2463	-4.69541	-0.20226
H	0.91258	-5.2685	1.33427
H	-0.38389	-4.06808	1.32519
C	2.65545	-3.80175	-1.53078
H	3.32598	-4.65721	-1.38101
H	1.69724	-4.18107	-1.8899
H	3.08548	-3.1771	-2.31609
C	1.15607	-2.45219	3.22361
H	0.08832	-2.6458	3.10484
H	1.57326	-3.27085	3.82554
H	1.27155	-1.52549	3.78503
C	3.71043	-0.64208	2.43307
H	3.10556	-0.33464	3.28608
H	4.62412	-1.10867	2.82094
H	4.00933	0.25442	1.88375
C	4.55632	-1.43656	-0.51452
H	4.42028	-1.45562	-1.59724
H	4.80413	-0.41576	-0.21996
H	5.41956	-2.07273	-0.27676
N	-2.25569	-0.44305	0.76301
O	0.19847	-0.22523	-1.03718
C	-0.03113	1.37104	0.74411
C	1.02015	0.96753	-0.03936
C	1.9641	1.78417	-0.7853
C	2.25137	1.55111	-2.15233
C	2.6369	2.84141	-0.12473
C	3.16063	2.35795	-2.82956
H	1.72374	0.76051	-2.67649
C	3.55849	3.62948	-0.80425
H	2.41603	3.03748	0.91987
C	3.82327	3.3901	-2.15772
H	3.35276	2.1857	-3.88415
H	4.06551	4.43719	-0.28556
H	4.53899	4.0111	-2.68764
C	-0.80737	2.58559	0.3883
C	-0.92956	3.01064	-0.95181
C	-1.47578	3.32148	1.38993
C	-1.66661	4.14535	-1.27164
H	-0.47584	2.42753	-1.74382
C	-2.19527	4.46783	1.06496
H	-1.41163	3.00687	2.42502
C	-2.29439	4.884	-0.26469
H	-1.76225	4.44809	-2.3097
H	-2.68433	5.03438	1.85136
H	-2.86727	5.77121	-0.51655
C	-3.53546	-0.4532	0.64119
H	-4.18616	-0.15081	1.47546
C	-4.22128	-0.84112	-0.58879
C	-3.50939	-1.2086	-1.74753
C	-5.62657	-0.84548	-0.60814
C	-4.2026	-1.57531	-2.89564
H	-2.42362	-1.1921	-1.73149
C	-6.31512	-1.21697	-1.76093
H	-6.17638	-0.55843	0.28495
C	-5.60311	-1.58264	-2.90518
H	-3.65403	-1.85514	-3.79017
H	-7.40062	-1.22048	-1.76856
H	-6.13735	-1.87101	-3.80573

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Sum of electronic and thermal Free Energies: -1669.813040

C	-0.81148	-0.38028	2.15621
C	-1.41588	-0.9474	3.29468
H	-2.49903	-0.95301	3.36996
C	-0.61846	-1.51085	4.27404
C	0.78383	-1.5144	4.12419
H	1.40431	-1.94307	4.9051
C	1.38592	-0.96423	3.00739
C	0.61251	-0.35951	1.97498

H	2.46395	-0.96051	2.92561
C	0.42168	-1.6614	-2.15999
C	0.95299	-2.67316	-1.28578
C	-0.16331	-3.43486	-0.74554
C	-1.37059	-2.86963	-1.22719
C	-1.01644	-1.73482	-2.07235
Rh	-0.25475	-1.21635	-0.07871
H	-1.07303	-1.95232	5.15593
C	-2.75934	-3.39044	-1.00998
H	-3.49278	-2.58265	-0.95542
H	-3.05562	-4.03967	-1.84366
H	-2.83381	-3.97928	-0.09322
C	-1.98634	-0.9293	-2.87909
H	-2.29355	-1.50182	-3.76334
H	-2.88644	-0.68667	-2.31161
H	-1.54671	0.00738	-3.22796
C	-0.01209	-4.63377	0.13665
H	-0.92468	-4.85394	0.69399
H	0.22654	-5.51486	-0.4733
H	0.80697	-4.50353	0.84884
C	2.38841	-3.07838	-1.16589
H	2.65989	-3.31799	-0.13702
H	2.5616	-3.9679	-1.78499
H	3.0655	-2.29399	-1.50247
C	1.21323	-0.79365	-3.08968
H	0.67459	0.11837	-3.35593
H	2.1781	-0.50768	-2.66711
H	1.40968	-1.34062	-4.02117
N	-1.59468	0.08228	1.07483
O	3.02828	-1.06584	0.8204
C	1.11612	0.33242	0.74788
C	2.56578	0.00787	0.43016
C	3.52399	0.94548	-0.25643
C	4.86934	0.83045	0.14977
C	3.21576	1.83587	-1.29791
C	5.8667	1.59382	-0.44808
H	5.11559	0.1324	0.94117
C	4.22268	2.58062	-1.91454
H	2.1986	1.95168	-1.643
C	5.54765	2.46716	-1.48984
H	6.89451	1.49889	-0.11044
H	3.96784	3.2501	-2.73024
H	6.32629	3.05468	-1.96794
C	0.67089	1.77204	0.58766
C	0.85142	2.67574	1.64592
C	0.07658	2.24788	-0.59103
C	0.46123	4.01274	1.52363
H	1.30476	2.33411	2.57237
C	-0.30078	3.58246	-0.72426
H	-0.1081	1.54996	-1.40274
C	-0.11013	4.4731	0.3364
H	0.60946	4.69523	2.35636
H	-0.7562	3.92313	-1.64977
H	-0.40626	5.51267	0.23699
C	-2.38868	1.08523	1.212
H	-2.29895	1.67526	2.13315
C	-3.44064	1.50908	0.29078
C	-4.29058	0.57122	-0.32479
C	-3.70936	2.88692	0.15147
C	-5.3834	1.00489	-1.07347
H	-4.12876	-0.48433	-0.14657
C	-4.77781	3.31573	-0.63076
H	-3.06278	3.61174	0.6384
C	-5.6239	2.37699	-1.23326
H	-6.06379	0.27837	-1.51036
H	-4.96292	4.37326	-0.75774
H	-6.47929	2.71317	-1.81051

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Sum of electronic and thermal Free Energies: -2016.692391

C	-0.99767	-0.03817	2.14782
C	-1.47355	-0.7063	3.27883
H	-2.54125	-0.87991	3.36601
C	-0.60603	-1.19726	4.25145
C	0.76427	-1.02764	4.07648
H	1.46328	-1.40039	4.81875
C	1.25372	-0.36254	2.95657
C	0.41151	0.17807	1.94184
H	2.31234	-0.18709	2.86437
C	3.20717	-1.25411	-0.86583
C	3.08054	-2.07139	0.3066
C	2.15631	-3.17213	0.01077
C	1.66261	-2.97536	-1.28991
C	2.22777	-1.72708	-1.81213
Rh	1.11098	-1.09414	-0.0518
H	-1.00036	-1.71633	5.11922
C	0.779	-3.89237	-2.07097
H	0.06762	-3.3402	-2.69041
H	1.39521	-4.49498	-2.75087

H	0.22329	-4.57024	-1.42454
C	2.02731	-1.21728	-3.20466
H	2.67067	-1.76745	-3.90417
H	0.99431	-1.35109	-3.53464
H	2.27994	-0.1582	-3.28542
C	1.84105	-4.30131	0.93859
H	0.86631	-4.73678	0.71865
H	2.60375	-5.08621	0.85289
H	1.82881	-3.96701	1.97856
C	3.97207	-2.00729	1.50528
H	3.49832	-2.44515	2.38584
H	4.88353	-2.58519	1.30089
H	4.26395	-0.98188	1.73449
C	4.28324	-0.24835	-1.11582
H	4.0123	0.46859	-1.89109
H	4.54887	0.30317	-0.21235
H	5.18031	-0.78343	-1.45534
N	-1.95635	0.33641	1.16173
O	3.19655	1.11318	1.6735
C	0.95573	0.94355	0.75491
C	2.36476	1.50985	0.85211
C	2.82638	2.6321	-0.04995
C	3.68942	3.57374	0.53756
C	2.55116	2.7408	-1.42228
C	4.22911	4.6146	-0.21432
H	3.92944	3.47696	1.5907
C	3.11616	3.76541	-2.18083
H	1.90523	2.02035	-1.90665
C	3.94658	4.71236	-1.57817
H	4.87743	5.3436	0.26231
H	2.90325	3.8267	-3.24405
H	4.37365	5.51748	-2.16849
C	0.01843	1.9727	0.13845
C	-0.25987	3.13141	0.88264
C	-0.49647	1.88482	-1.16105
C	-1.02041	4.16905	0.34486
H	0.13654	3.22659	1.89069
C	-1.24707	2.9288	-1.70865
H	-0.29964	0.9955	-1.75179
C	-1.51011	4.07575	-0.9599
H	-1.21479	5.05778	0.93821
H	-1.62079	2.84589	-2.72548
H	-2.08879	4.88889	-1.38717
C	-2.98809	1.03357	1.51338
H	-3.03952	1.36812	2.55309
C	-4.10012	1.44505	0.6736
C	-4.11962	1.28474	-0.72572
C	-5.20093	2.05059	1.31084
C	-5.22026	1.70932	-1.46038
H	-3.26025	0.85771	-1.22688
C	-6.30463	2.46643	0.57221
H	-5.18738	2.18791	2.38879
C	-6.31532	2.29498	-0.81403
H	-5.22846	1.59015	-2.53927
H	-7.15083	2.92581	1.07261
H	-7.17299	2.62292	-1.3934
H	-1.60531	-0.4347	0.00606
O	-1.18155	-1.10248	-0.60589
C	-1.70947	-2.35686	-0.41206
O	-1.19304	-3.13211	0.36579
C	-2.9792	-2.71214	-1.2106
C	-4.19264	-2.32262	-0.32864
H	-4.23654	-1.24905	-0.13266
H	-5.11799	-2.60165	-0.84226
H	-4.16294	-2.85314	0.6277
C	-3.01549	-4.23643	-1.43937
H	-3.95736	-4.51077	-1.92397
H	-2.1997	-4.56609	-2.0896
H	-2.93879	-4.77883	-0.49531
C	-3.03915	-1.98006	-2.56305
H	-2.1894	-2.2466	-3.20054
H	-3.95163	-2.26716	-3.09495
H	-3.04064	-0.89496	-2.44733

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Sum of electronic and thermal Free Energies: -2016.692123

C	-1.00601	-0.04888	2.13549
C	-1.47775	-0.73187	3.25956
H	-2.54494	-0.9086	3.34642
C	-0.60838	-1.23306	4.22558
C	0.76131	-1.05894	4.05245
H	1.46156	-1.43901	4.78979
C	1.24807	-0.3785	2.94048
C	0.4039	0.17255	1.93239
H	2.3058	-0.19692	2.85116
C	3.22111	-1.23748	-0.85991
C	3.09746	-2.05452	0.31391
C	2.18054	-3.16109	0.01834
C	1.68696	-2.96761	-1.28294

C	2.24703	-1.71729	-1.80696
Rh	1.12374	-1.08887	-0.04649
H	-1.00147	-1.76301	5.08737
C	0.81017	-3.8908	-2.06466
H	0.10016	-3.34395	-2.69044
H	1.43226	-4.49371	-2.73893
H	0.2536	-4.56839	-1.4186
C	2.04533	-1.21073	-3.20059
H	2.68877	-1.76135	-3.89964
H	1.01224	-1.34626	-3.5297
H	2.29643	-0.15146	-3.28354
C	1.87051	-4.29178	0.94636
H	0.89861	-4.73313	0.72504
H	2.6373	-5.07282	0.86222
H	1.85469	-3.9572	1.98621
C	3.9886	-1.98331	1.51259
H	3.52127	-2.43104	2.39157
H	4.90766	-2.54799	1.30531
H	4.26737	-0.95501	1.74577
C	4.29094	-0.22439	-1.10719
H	4.01774	0.4897	-1.88426
H	4.54912	0.33027	-0.20343
H	5.19337	-0.75311	-1.44244
N	-1.96626	0.33196	1.1548
O	3.18293	1.13459	1.68884
C	0.94975	0.94909	0.75441
C	2.35456	1.52476	0.86102
C	2.81473	2.6488	-0.03937
C	3.66925	3.59584	0.55198
C	2.54609	2.75493	-1.41321
C	4.20681	4.63926	-0.19784
H	3.90418	3.50123	1.60647
C	3.10901	3.78229	-2.16951
H	1.90704	2.03025	-1.90038
C	3.93077	4.73447	-1.56321
H	4.84837	5.37235	0.28165
H	2.90123	3.84167	-3.23386
H	4.35615	5.54171	-2.15184
C	0.00937	1.97074	0.13084
C	-0.27908	3.12971	0.87068
C	-0.49817	1.87695	-1.17114
C	-1.04253	4.16183	0.32645
H	0.11146	3.22954	1.88057
C	-1.25189	2.91523	-1.72504
H	-0.29257	0.98795	-1.75939
C	-1.52513	4.06257	-0.98044
H	-1.24495	5.05083	0.91669
H	-1.61978	2.82785	-2.74364
H	-2.10624	4.87136	-1.41263
C	-2.99891	1.02003	1.51956
H	-3.05034	1.34496	2.56279
C	-4.11731	1.43265	0.68707
C	-4.13898	1.28725	-0.71364
C	-5.22184	2.02123	1.33311
C	-5.2453	1.70939	-1.44131
H	-3.27604	0.87499	-1.22113
C	-6.33138	2.43467	0.60159
H	-5.20689	2.1472	2.41246
C	-6.34425	2.27783	-0.78627
H	-5.25483	1.60215	-2.52147
H	-7.18042	2.88096	1.109
H	-7.20635	2.60403	-1.36003
H	-1.62768	-0.41197	0.01782
O	-1.13967	-1.16102	-0.65822
C	-1.67262	-2.41929	-0.47063
O	-1.15493	-3.19711	0.30152
C	-2.93998	-2.7663	-1.27442
C	-4.1552	-2.3815	-0.39267
H	-4.19847	-1.30919	-0.18978
H	-5.07912	-2.65632	-0.91103
H	-4.12873	-2.91853	0.5601
C	-2.97558	-4.28895	-1.51446
H	-3.91507	-4.55919	-2.00578
H	-2.15636	-4.61391	-2.16281
H	-2.90401	-4.83839	-0.57405
C	-2.99487	-2.02325	-2.62113
H	-2.14217	-2.28365	-3.25721
H	-3.9049	-2.30712	-3.15882
H	-2.99859	-0.93909	-2.49633

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Sum of electronic and thermal Free Energies: -2016.726645

C	0.57066	1.14279	2.25285
C	-0.22723	1.47713	3.34669
H	-0.84236	2.37033	3.30687
C	-0.22294	0.66266	4.47628
C	0.55628	-0.49489	4.47775
H	0.55293	-1.15193	5.34221
C	1.33343	-0.82479	3.36679

C	1.38519	-0.00845	2.22127
H	1.89497	-1.75237	3.37255
C	-1.64692	-3.04214	-1.02592
C	-1.58642	-3.05117	0.39777
C	-2.77658	-2.36142	0.89958
C	-3.59614	-1.99339	-0.22508
C	-2.87425	-2.34906	-1.41067
Rh	-1.58581	-0.97123	-0.28097
H	-0.83064	0.92403	5.33598
C	-4.97157	-1.40701	-0.16424
H	-5.22355	-0.87746	-1.0861
H	-5.70383	-2.21481	-0.03725
H	-5.06795	-0.70891	0.66669
C	-3.33094	-2.1355	-2.81806
H	-3.88977	-3.01572	-3.16177
H	-3.99111	-1.2699	-2.90108
H	-2.48778	-1.99519	-3.49825
C	-3.13416	-2.16162	2.33533
H	-3.60277	-1.18581	2.47287
H	-3.83815	-2.94277	2.65204
H	-2.25481	-2.22018	2.98015
C	-0.53323	-3.69124	1.24586
H	-0.35053	-3.11628	2.15661
H	-0.85781	-4.69645	1.54594
H	0.41209	-3.78947	0.70707
C	-0.69339	-3.6961	-1.97498
H	-0.56493	-3.11297	-2.8892
H	0.29379	-3.83448	-1.53294
H	-1.08131	-4.68293	-2.25877
N	0.48771	1.96899	1.07654
O	0.26796	-0.208	-0.27542
C	2.20417	-0.39743	1.02798
C	1.51723	-0.65556	-0.14434
C	2.06111	-1.3857	-1.32617
C	2.85609	-2.53499	-1.17332
C	1.70965	-0.97604	-2.62326
C	3.29603	-3.24728	-2.28883
H	3.13273	-2.86386	-0.17634
C	2.162	-1.68192	-3.73913
H	1.0918	-0.09231	-2.74805
C	2.95406	-2.82122	-3.5758
H	3.90762	-4.13467	-2.15367
H	1.89956	-1.34109	-4.73696
H	3.30424	-3.37246	-4.44373
C	3.69103	-0.40748	1.13949
C	4.37107	-0.7229	2.3335
C	4.48076	0.00477	0.04049
C	5.7648	-0.67197	2.40886
H	3.8194	-1.00141	3.22168
C	5.86996	0.03859	0.11557
H	3.99632	0.30998	-0.88346
C	6.52485	-0.3028	1.2996
H	6.25351	-0.92162	3.34368
H	6.44268	0.35	-0.75378
H	7.60953	-0.26762	1.35926
C	1.49842	2.64816	0.62649
H	2.36326	2.7048	1.28419
C	1.56617	3.32342	-0.64775
C	0.62669	3.10655	-1.67773
C	2.63991	4.21371	-0.85358
C	0.76756	3.78132	-2.88228
H	-0.18804	2.40263	-1.53627
C	2.76086	4.89619	-2.05821
H	3.36256	4.37398	-0.05728
C	1.82684	4.67759	-3.07217
H	0.05785	3.60738	-3.68582
H	3.58117	5.58959	-2.2094
H	1.92666	5.2029	-4.01912
H	-0.35801	1.80127	0.49802
O	-1.98368	1.1097	-0.15996
C	-3.06322	1.55119	0.47245
O	-3.63893	0.91475	1.34865
C	-3.55574	2.9566	0.0437
C	-2.55671	4.01553	0.56106
H	-1.56879	3.9027	0.10479
H	-2.91854	5.01914	0.31508
H	-2.45041	3.96254	1.65016
C	-4.9388	3.22002	0.66251
H	-5.29573	4.21395	0.37021
H	-5.67196	2.48135	0.32305
H	-4.90126	3.16892	1.75322
C	-3.64531	3.03648	-1.49418
H	-4.36281	2.30795	-1.88729
H	-3.98591	4.03159	-1.79868
H	-2.67695	2.84447	-1.96265

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Sum of electronic and thermal Free Energies: -2016.710387

C	0.76081439	0.93758835	-2.58841600

C	-0.03853361	1.02739835	-3.72335600	C	1.23490808	-1.81243253	3.62964548
H	-0.61211861	1.92843435	-3.91465300	H	0.05114827	-2.02482652	1.83882002
C	-0.07209461	-0.05262965	-4.61092400	C	2.45934917	-1.39972771	4.16386335
C	0.68278739	-1.19808865	-4.35234900	H	4.39630711	-0.55148694	3.73700164
H	0.66209039	-2.03054865	-5.04938500	H	0.46206429	-2.20699034	4.28276923
C	1.47888039	-1.27780665	-3.20134300	H	2.64267988	-1.48339102	5.23086986
C	1.54094339	-0.20177865	-2.31460900	C	3.79237386	-0.26218736	-1.00682028
H	2.05106039	-2.17966465	-3.00472100	C	4.45220306	-1.49937160	-1.12744342
C	2.22050782	-5.26962780	-0.56682805	C	4.59124533	0.90117868	-1.01372729
C	1.83276162	-5.17077421	-1.93434954	C	5.84423794	-1.57407997	-1.20515268
C	0.49534913	-5.74948331	-2.07945376	H	3.87976115	-2.41767703	-1.17038421
C	0.06655205	-6.20487164	-0.78972162	C	5.98010243	0.82429872	-1.08872467
C	1.10914110	-5.85914941	0.15685835	H	4.12555570	1.87790282	-0.96802705
Rh	0.38096018	-4.02308137	-0.73625133	C	6.61763079	-0.41510799	-1.17777480
H	-0.67847061	0.00895835	-5.50921600	H	6.32031157	-2.54631875	-1.29153217
C	-1.17289486	-6.98363274	-0.48825392	H	6.56514801	1.73942195	-1.08666301
H	-1.47479171	-6.87212367	0.55533445	H	7.70001958	-0.47369126	-1.23717729
H	-0.97892669	-8.04942798	-0.66495864	C	1.33788646	1.50609741	-0.37245155
H	-2.00060786	-6.66392080	-1.12056504	H	2.24748629	2.06914850	-0.17245223
C	1.09331120	-6.15150322	1.62108036	C	0.36382395	1.52764676	0.73307855
H	1.56592487	-7.12571943	1.80390538	C	-0.94458124	1.02297354	0.60209069
H	0.07585131	-6.19858374	2.01327159	C	0.75371645	2.09650855	1.95929158
H	1.65140405	-5.40195253	2.18636148	C	-1.83206580	1.09333789	1.67439820
C	-0.24476839	-5.91505852	-3.36408888	H	-1.27075488	0.57398102	-0.33076235
H	-1.30736903	-5.71867931	-3.21584530	C	-0.13701299	2.15854002	3.02925222
H	-0.11768454	-6.94413311	-3.72565941	H	1.75633897	2.49896615	2.06599285
H	0.13392567	-5.24073757	-4.13451644	C	-1.43256638	1.65770748	2.88925508
C	2.65064932	-4.62791583	-3.06135549	H	-2.84330871	0.71380459	1.55999788
H	2.05788821	-3.98558034	-3.71791310	H	0.17645935	2.60749250	3.96656812
H	3.03681913	-5.45745313	-3.66694016	H	-2.13081111	1.71458862	3.71880580
H	3.50350640	-4.05155992	-2.70004746	H	-0.02595061	2.00511335	-1.02641100
C	3.54196886	-4.89444701	0.02547061	O	-1.45453192	-3.16203583	-0.44417926
H	3.44417358	-4.53090950	1.04976679	C	-2.58270995	-3.71783235	-0.87115515
H	4.04525631	-4.12019469	-0.55464820	O	-2.61942048	-4.57944513	-1.74352068
H	4.19395251	-5.77693240	0.04391527	C	-3.86760343	-3.18933846	-0.19262057
N	0.82699939	1.93624335	-1.58008100	C	-4.05312070	-1.69411142	-0.53268836
O	0.97506986	-2.02955913	-0.54440193	H	-3.25732658	-1.07511343	-0.11129887
C	2.29500139	-0.17516065	-0.99917500	H	-5.00093945	-1.33685073	-0.11730099
C	1.75638460	-1.14718361	-0.06024318	H	-4.08644410	-1.53257519	-1.61552898
C	1.97841060	-1.16054531	1.41230330	C	-5.07621973	-3.98514091	-0.71235110
C	3.20199359	-0.73723663	1.95864082	H	-5.99189834	-3.62210061	-0.23463734
C	1.00110121	-1.71165659	2.25850599	H	-4.97472377	-5.05158015	-0.49384803
C	3.44405987	-0.87098237	3.32508410	H	-5.18517121	-3.87981276	-1.79439470
H	3.96112173	-0.30787884	1.31396335	C	-3.74115089	-3.36566912	1.33614997

H	-3.62720680	-4.42195773	1.60511297
H	-4.64534664	-2.99546071	1.83021205
H	-2.88394876	-2.81638213	1.73344658

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Sum of electronic and thermal Free Energies: -2016.728943

C	-0.89443600	0.90507100	1.68957300
C	-3.88493100	2.57431300	-0.87634600
C	-4.02448700	3.89894800	-1.29626700
C	-2.90515500	4.65155500	-1.65212900
C	-1.63967800	4.06565400	-1.59737300
C	-1.49614000	2.74130500	-1.18386500
C	-2.53817300	-0.32256700	-1.71118100
C	-1.67075400	-0.43868200	-2.79267400
C	-2.06702800	-1.18330400	-3.91143800
C	-3.33230900	-1.77966800	-3.94527600
C	-4.22524800	-1.63856100	-2.88047500
C	-1.64300100	1.99367800	2.17886000
C	-3.81619900	-0.89670800	-1.76931500
C	-3.65242200	-0.09924100	0.42577100
C	-3.31245400	-1.20591300	1.42359600
C	-2.87899800	-2.47400700	1.00117200
C	-2.62653100	-3.48458400	1.93048700
C	-2.80454400	-3.24844100	3.29668600
C	-3.24694200	-1.99678400	3.72574700
C	-3.50236400	-0.98851700	2.79464300
C	-1.40305000	2.49445700	3.45600900
C	-0.43290900	1.90910400	4.27256000
C	0.30244400	0.81533600	3.80689000
C	0.07646100	0.32359500	2.52676000
C	-1.10668000	0.32418100	0.34296400
C	-2.43463800	0.49520600	-0.41850700
C	-2.61559400	1.98243100	-0.80533700
H	-5.25205100	-1.25409200	-0.32784000
H	-4.77163500	1.99676300	-0.63959600
H	-5.01595500	4.33863400	-1.34997200
H	-3.01827900	5.68180700	-1.97498900
H	-0.75974900	4.63758600	-1.87639700
H	-0.50089700	2.30578000	-1.15109500
H	-0.70281000	0.05072100	-2.77659700
H	-1.40180400	-1.27667800	-4.76447100
H	-3.63478900	-2.35110200	-4.81781900
H	-5.21440200	-2.08463100	-2.91987200
H	-4.12524800	0.71471800	0.98200100
H	-2.75845500	-2.67815900	-0.05799600
H	-2.31730200	-4.46808100	1.58611600
H	-2.61986700	-4.03964900	4.01717700
H	-3.40757100	-1.80763400	4.78285000
H	-3.85578600	-0.02020400	3.13848500
H	-2.38517300	2.47160000	1.55277300
H	-1.97212700	3.34719500	3.81225300
H	-0.25294200	2.30018200	5.26935500
H	1.04448500	0.34673600	4.44580300
H	0.62843600	-0.54231700	2.17826100
N	-4.56171200	-0.57729600	-0.63077600
O	-0.22390800	-0.35153200	-0.21511100
C	1.68535300	-2.94062200	-0.72024800
C	2.36339300	-2.78811000	0.52783200
C	3.60917800	-2.04897300	0.29481300
C	3.67760700	-1.73409700	-1.09819500
C	2.46397400	-2.25101300	-1.72100400
Rh	1.89853500	-0.77710900	-0.23394400
C	4.82245000	-1.08081200	-1.80059400
H	4.52885700	-0.69479500	-2.77862200
H	5.61921000	-1.81882600	-1.95946800
H	5.21715700	-0.25679900	-1.20500700
C	2.11954300	-2.15509600	-3.17004600
H	2.55861200	-3.00932800	-3.70280100
H	2.51976000	-1.24515400	-3.62202800
H	1.03984600	-2.18223900	-3.33060200
C	4.66423900	-1.74804400	1.30670300
H	5.03199000	-0.72890700	1.17191000
H	5.50133600	-2.44650400	1.17868900
H	4.29351200	-1.85704400	2.32746000
C	1.92212800	-3.33834000	1.84578800
H	2.28498000	-2.73173200	2.67813200
H	2.33223600	-4.34832700	1.97497700
H	0.83460600	-3.40884300	1.91624700
C	0.37957600	-3.62998500	-0.96562900
H	-0.26853800	-3.03403600	-1.61382300
H	-0.15752100	-3.81289900	-0.03407000
H	0.55208500	-4.59654800	-1.45373000
O	2.11896600	1.19916300	-0.08198500
C	3.28326900	1.82664700	0.07154200
O	4.34562200	1.24165300	0.24973000
C	3.17646600	3.36202500	0.00136300
C	2.10894100	3.85307800	1.00250300
H	1.12322200	3.44316900	0.77218100
H	2.04605100	4.94573600	0.96705300

H	2.36653700	3.56804300	2.02820300
C	4.54099800	3.98459100	0.33598900
H	4.47615800	5.07550900	0.27068000
H	5.31526000	3.64217400	-0.35485200
H	4.86046800	3.72041900	1.34785400
C	2.76055300	3.74609400	-1.43757200
H	3.50697100	3.41578200	-2.16821100
H	2.67475700	4.83455200	-1.52027000
H	1.79741800	3.30290200	-1.70514900

P

Sum of electronic and thermal Free Energies: -1171.144813

C	-1.63315300	1.13577500	0.83028300
C	1.85272900	1.65888200	-1.62470200
C	2.48968900	2.85820800	-1.94923700
C	2.63726200	3.86327200	-0.99313900
C	2.15183400	3.65312900	0.29812300
C	1.51684200	2.45496000	0.62427900
C	1.81992900	-0.82895600	0.53262200
C	2.57349400	-0.84215700	1.70022100
C	3.61544700	-1.76989800	1.82886300
C	3.89906900	-2.65921400	0.78922400
C	3.15538900	-2.64517500	-0.39485200
C	-1.81786700	1.88196900	-0.34444900
C	2.11673600	-1.72033800	-0.50780100
C	0.11203500	-0.70522100	-1.16581600
C	-1.10269600	-1.58774000	-0.89372400
C	-1.09570400	-2.58338600	0.09779100
C	-2.20316000	-3.41174400	0.27627300
C	-3.33259600	-3.26710900	-0.53319600
C	-3.34836700	-2.28563700	-1.52415700
C	-2.24040200	-1.45514500	-1.70024300
C	-3.00765200	2.57744500	-0.55841400
C	-4.02835300	2.53394100	0.39280100
C	-3.85334800	1.79605100	1.56677600
C	-2.66411300	1.10756800	1.78450900
C	-0.38873000	0.35433900	1.15632400
C	0.69355200	0.10288200	0.07261700
C	1.34524000	1.44350800	-0.33411700
H	1.02266900	-2.33843200	-2.13491400
H	1.78322700	0.87519700	-2.37148700
H	2.87722900	3.00116600	-2.95420800
H	3.13071400	4.79642100	-1.24890300
H	2.26531000	4.42246900	1.05672100
H	1.15372300	2.30934900	1.63743800
H	2.34269900	-0.15964300	2.50950900
H	4.20161400	-1.79836000	2.74221000
H	4.70800900	-3.37637500	0.89889600
H	3.37889500	-3.33523800	-1.20359000
H	-0.16231000	-0.00412100	-1.95891900
H	-0.22815600	-2.70377500	0.73802800
H	-2.18356900	-4.17197300	1.05198500
H	-4.19301500	-3.91481100	-0.39127400
H	-4.22061900	-2.16454800	-2.16030200
H	-2.26015200	-0.68928300	-2.47165400
H	-1.02774100	1.94869400	-1.08255000
H	-3.13401800	3.15931100	-1.46680900
H	-4.95461200	3.07548500	0.22207700
H	-4.64431800	1.75907600	2.31028200
H	-2.50654500	0.53150600	2.68963100
N	1.27513800	-1.50830400	-1.61047300
O	-0.23170500	-0.07815700	2.28750000

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Sum of electronic and thermal Free Energies: -1669.813016

C	-1.38634	-0.61852	1.23329
C	-2.2041	-1.35794	2.11823
H	-3.12223	-1.80098	1.74772
C	-1.81789	-1.49677	3.43572
C	-0.61157	-0.91832	3.88946
H	-0.33062	-1.01914	4.93308
C	0.21227	-0.22025	3.0302
C	-0.14013	-0.03155	1.6621
H	1.13284	0.21271	3.39479
C	2.36011	-1.99732	-0.99215
C	1.9572	-2.90339	0.04674
C	0.75698	-3.59708	-0.38715
C	0.37907	-3.05805	-1.64886
C	1.35769	-2.04334	-2.02888
Rh	0.35254	-1.33877	-0.20978
H	-2.44371	-2.05414	4.12557
C	-0.7781	-3.48914	-2.49718
H	-1.21836	-2.64432	-3.03407
H	-0.44369	-4.21359	-3.2501
H	-1.56366	-3.96527	-1.90606
C	1.42856	-1.36092	-3.36068
H	1.93264	-2.00712	-4.09132
H	0.43492	-1.13613	-3.75704
H	1.99326	-0.42795	-3.30524
C	0.06765	-4.69507	0.36465

H	-0.97021	-4.81566	0.04702
H	0.57842	-5.65062	0.19228
H	0.07243	-4.51377	1.44236
C	2.71834	-3.15769	1.31088
H	2.11139	-3.69109	2.04503
H	3.60384	-3.77137	1.10303
H	3.04754	-2.21631	1.75453
C	3.65322	-1.24649	-1.03304
H	3.59838	-0.36259	-1.67208
H	3.96569	-0.92857	-0.03669
H	4.43604	-1.90159	-1.43727
N	-1.60921	-0.56361	-0.15608
O	2.65493	0.13149	1.75272
C	0.64089	0.70583	0.62427
C	2.09915	0.90728	0.96766
C	2.91531	2.05403	0.44454
C	3.85263	2.59831	1.34145
C	2.86835	2.55303	-0.86745
C	4.68879	3.6398	0.95104
H	3.91053	2.19409	2.34665
C	3.72968	3.57538	-1.26562
H	2.17351	2.14112	-1.58621
C	4.63101	4.13047	-0.35641
H	5.39053	4.06347	1.66274
H	3.69113	3.94236	-2.28731
H	5.28791	4.9381	-0.66519
C	-0.08979	1.8512	-0.05094
C	-0.59656	2.89269	0.74097
C	-0.27574	1.93002	-1.43962
C	-1.25525	3.98166	0.16357
H	-0.46517	2.85838	1.81962
C	-0.93182	3.01444	-2.02034
H	0.09305	1.12204	-2.06548
C	-1.42472	4.04722	-1.21908
H	-1.63269	4.77859	0.79698
H	-1.06094	3.05322	-3.09854
H	-1.93646	4.89234	-1.66967
C	-2.63871	-0.23416	-0.8569
H	-2.52568	-0.41231	-1.92656
C	-3.90113	0.39558	-0.47525
C	-4.18467	0.932	0.80033
C	-4.86464	0.52664	-1.49641
C	-5.40218	1.55744	1.0373
H	-3.45334	0.87639	1.59524
C	-6.08274	1.15111	-1.25234
H	-4.64673	0.13996	-2.48873
C	-6.35595	1.66349	0.01841
H	-5.61027	1.96985	2.02161
H	-6.81426	1.24331	-2.04893
H	-7.30439	2.15468	0.21427

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Sum of electronic and thermal Free Energies: -2016.691769

C	1.62087	0.08423	1.33256
C	2.10535	0.71455	2.48034
H	3.10365	1.13831	2.4425
C	1.34795	0.81875	3.65157
C	0.06967	0.28965	3.68522
H	-0.52637	0.33278	4.59061
C	-0.44352	-0.36515	2.55497
C	0.30176	-0.51277	1.33411
H	-1.35754	-0.92696	2.6626
C	-3.54346	0.60966	1.05841
C	-3.08922	1.82843	1.7611
C	-2.63321	2.7368	0.79701
C	-2.82929	2.11821	-0.52742
C	-3.49913	0.86854	-0.36366
Rh	-1.44641	0.74826	0.55727
H	1.77345	1.30512	4.52388
C	-2.54523	2.80336	-1.8231
H	-2.47147	2.09203	-2.64856
H	-3.37258	3.48942	-2.05239
H	-1.62952	3.3965	-1.7713
C	-4.1427	0.05346	-1.43884
H	-5.18049	0.38734	-1.57082
H	-3.63667	0.17411	-2.39868
H	-4.16238	-1.00975	-1.19937
C	-2.09253	4.11237	1.02463
H	-1.27782	4.34178	0.33405
H	-2.88597	4.85342	0.85941
H	-1.73386	4.23848	2.0486
C	-3.15659	2.04229	3.24042
H	-2.37841	2.72465	3.58802
H	-4.12667	2.48313	3.50406
H	-3.06558	1.10538	3.79332
C	-4.23014	-0.5495	1.70722
H	-4.177	-1.45005	1.09266
H	-3.80999	-0.78108	2.68829
H	-5.29104	-0.30597	1.85492

N	2.41254	0.20161	0.17317
O	-1.36132	-2.76315	1.63538
C	-0.38285	-1.13957	0.16609
C	-1.28349	-2.33791	0.48397
C	-2.08445	-3.05655	-0.57682
C	-2.75252	-4.22084	-0.14679
C	-2.22266	-2.67006	-1.92201
C	-3.52675	-4.97141	-1.02582
H	-2.643	-4.52176	0.8885
C	-3.00207	-3.42247	-2.80116
H	-1.72001	-1.79004	-2.29656
C	-3.65376	-4.5749	-2.3596
H	-4.02737	-5.86795	-0.67294
H	-3.09254	-3.10936	-3.83706
H	-4.25256	-5.16156	-3.04998
C	0.38251	-1.30006	-1.12871
C	1.11635	-2.48094	-1.33103
C	0.3645	-0.34568	-2.15609
C	1.82681	-2.69062	-2.51263
H	1.13688	-3.24038	-0.55443
C	1.06894	-0.55587	-3.34272
H	-0.20294	0.56959	-2.02328
C	1.80573	-1.72805	-3.52432
H	2.38916	-3.60997	-2.64581
H	1.03686	0.19414	-4.12777
H	2.34943	-1.89467	-4.44932
C	3.50277	-0.43483	-0.0708
H	4.03301	-0.09138	-0.96233
C	4.16667	-1.55168	0.61241
C	3.58996	-2.33452	1.63295
C	5.4684	-1.86375	0.17309
C	4.30548	-3.38663	2.19606
H	2.58476	-2.13284	1.98038
C	6.18566	-2.90892	0.7476
H	5.91636	-1.27599	-0.62395
C	5.60382	-3.6727	1.76138
H	3.85002	-3.98782	2.97672
H	7.19036	-3.1316	0.40272
H	6.15673	-4.49305	2.2088
H	1.67729	1.72784	-0.53848
O	0.92936	2.37684	-0.60534
C	1.23435	3.5854	-1.13226
O	0.34594	4.40438	-1.26224
C	2.69507	3.84326	-1.53782
C	3.607	3.69233	-0.29828
H	3.59162	2.6778	0.1103
H	4.63994	3.92217	-0.57712
H	3.31351	4.38694	0.49521
C	2.80714	5.27369	-2.09015
H	3.83942	5.47108	-2.39472
H	2.1564	5.41626	-2.95596
H	2.52125	6.012	-1.33717
C	3.10388	2.82935	-2.63162
H	2.48222	2.94353	-3.52556
H	4.14342	3.00657	-2.92439
H	3.02239	1.7906	-2.29618

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Sum of electronic and thermal Free Energies: -2016.690537

C	-1.62465	-0.35729	1.32518
C	-2.24241	-1.07503	2.35445
H	-3.13538	-1.64597	2.12325
C	-1.72108	-1.07866	3.64399
C	-0.55587	-0.35837	3.90124
H	-0.13687	-0.33281	4.90252
C	0.07794	0.34536	2.88287
C	-0.40911	0.38183	1.54362
H	0.94974	0.93601	3.10803
C	3.62315	-0.10102	0.42343
C	3.25962	-0.86691	1.57859
C	2.96681	-2.24145	1.15974
C	3.0701	-2.28789	-0.24362
C	3.38007	-0.93872	-0.72579
Rh	1.45293	-0.72716	0.27701
H	-2.21668	-1.64138	4.42866
C	2.98208	-3.48857	-1.1291
H	2.45523	-3.26587	-2.06056
H	3.99775	-3.80411	-1.40144
H	2.47827	-4.32167	-0.64262
C	3.68757	-0.5959	-2.14906
H	4.70388	-0.92686	-2.40146
H	3.00191	-1.0932	-2.83935
H	3.63701	0.47974	-2.32476
C	2.64969	-3.3726	2.0846
H	2.09879	-4.15996	1.57088
H	3.57418	-3.79802	2.49607
H	2.04077	-3.03426	2.92683
C	3.42793	-0.42051	2.99544
H	2.74189	-0.93853	3.66819

H	4.45014	-0.6521	3.32371
H	3.27717	0.65517	3.09431
C	4.31091	1.22542	0.43851
H	4.24514	1.73738	-0.52144
H	3.91219	1.88805	1.20927
H	5.37401	1.05816	0.65706
N	-2.13848	-0.53639	0.01193
O	1.74426	2.34306	1.96142
C	0.288	1.14628	0.4358
C	1.26706	2.23545	0.82713
C	1.70131	3.28425	-0.17002
C	1.92952	4.57109	0.34669
C	1.98274	3.04499	-1.52434
C	2.39051	5.59795	-0.47414
H	1.74018	4.75241	1.39905
C	2.47206	4.06588	-2.33865
H	1.83265	2.05884	-1.94365
C	2.66654	5.34774	-1.81984
H	2.54245	6.5908	-0.06168
H	2.6969	3.86142	-3.38136
H	3.03432	6.14447	-2.45942
C	-0.61851	1.61633	-0.69619
C	-1.55351	2.62352	-0.40324
C	-0.54552	1.15064	-2.01628
C	-2.40472	3.1276	-1.38619
H	-1.61244	3.0191	0.60771
C	-1.39592	1.65084	-3.00319
H	0.16938	0.3753	-2.26785
C	-2.33343	2.63778	-2.69191
H	-3.11896	3.9056	-1.13326
H	-1.32178	1.27227	-4.01879
H	-2.99239	3.03003	-3.46061
C	-3.34682	-0.33965	-0.40271
H	-3.52542	-0.69304	-1.41883
C	-4.50486	0.29418	0.22169
C	-4.4595	1.11336	1.36928
C	-5.74238	0.09709	-0.42492
C	-5.62344	1.69856	1.85368
H	-3.51895	1.30145	1.87027
C	-6.90743	0.67023	0.07502
H	-5.78472	-0.5145	-1.32229
C	-6.8489	1.47244	1.21633
H	-5.57895	2.33443	2.73218
H	-7.85433	0.5004	-0.42704
H	-7.75393	1.92801	1.60635
H	-1.17064	-1.12778	-0.69436
O	-0.17833	-1.6778	-0.97747
C	-0.34856	-3.02959	-0.90992
O	0.16527	-3.69021	-0.03116
C	-1.23106	-3.66774	-2.00465
C	-2.55749	-4.09415	-1.32963
H	-3.11483	-3.23367	-0.94513
H	-3.19382	-4.60615	-2.05816
H	-2.3668	-4.77654	-0.49741
C	-0.50363	-4.93114	-2.51484
H	-1.1384	-5.45788	-3.23387
H	0.43239	-4.67573	-3.02303
H	-0.2729	-5.60824	-1.6902
C	-1.5056	-2.71921	-3.18333
H	-0.57768	-2.40748	-3.6719
H	-2.1214	-3.23102	-3.92954
H	-2.03646	-1.81227	-2.8801

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Sum of electronic and thermal Free Energies: -2016.729801

C	1.35808	1.47072	1.24638
C	1.24175	2.50262	2.18304
H	0.94525	3.49115	1.84675
C	1.51404	2.25838	3.52428
C	1.91263	0.97644	3.90933
H	2.14166	0.76678	4.94947
C	2.01056	-0.04423	2.96846
C	1.71124	0.14794	1.60286
H	2.32285	-1.02682	3.2976
C	-2.89251	-2.50688	0.2728
C	-2.63539	-1.94942	1.55782
C	-3.50912	-0.78494	1.72967
C	-4.32584	-0.65784	0.55694
C	-3.9037	-1.67508	-0.3681
Rh	-2.15284	-0.43366	0.05564
H	1.42131	3.05642	4.25292
C	-5.44175	0.31952	0.36125
H	-5.67436	0.45734	-0.69692
H	-6.34772	-0.05851	0.85158
H	-5.18971	1.29153	0.78634
C	-4.46186	-1.9183	-1.73291
H	-5.25475	-2.67568	-1.67654
H	-4.89607	-1.01321	-2.1613
H	-3.69651	-2.2943	-2.41608

C	-3.60122	0.07673	2.94568
H	-3.64216	1.12817	2.65325
H	-4.51284	-0.17064	3.50481
H	-2.74937	-0.07241	3.61147
C	-1.67756	-2.47048	2.58146
H	-1.24038	-1.65953	3.16845
H	-2.19905	-3.14197	3.27495
H	-0.86314	-3.03112	2.11852
C	-2.31028	-3.7566	-0.30803
H	-2.118	-3.65803	-1.37846
H	-1.36897	-4.0274	0.1705
H	-3.01396	-4.58688	-0.16699
N	1.08088	1.8182	-0.12531
O	-0.19199	-0.36867	-0.3904
C	1.82866	-0.98074	0.63351
C	0.8323	-1.22291	-0.28194
C	0.81731	-2.34532	-1.26986
C	1.28366	-3.63724	-0.97366
C	0.26231	-2.11079	-2.54131
C	1.20455	-4.65788	-1.92132
H	1.70842	-3.84712	0.00062
C	0.19404	-3.12939	-3.49174
H	-0.10603	-1.11827	-2.77947
C	0.66268	-4.40929	-3.18409
H	1.56754	-5.65041	-1.67068
H	-0.22084	-2.9234	-4.4745
H	0.60832	-5.20443	-3.9218
C	3.1288	-1.7347	0.62536
C	3.51288	-2.63723	1.63224
C	4.03243	-1.49822	-0.42485
C	4.76175	-3.26176	1.59972
H	2.81975	-2.88514	2.43472
C	5.27403	-2.13388	-0.46608
H	3.74859	-0.81027	-1.22145
C	5.64862	-3.01035	0.55312
H	5.03742	-3.95656	2.39182
H	5.94991	-1.93801	-1.29376
H	6.61828	-3.50148	0.52863
C	1.8872	2.33757	-1.00219
H	1.41352	2.51543	-1.96559
C	3.28414	2.70559	-0.91951
C	4.12414	2.51518	0.20247
C	3.82952	3.27576	-2.09549
C	5.46175	2.88451	0.13314
H	3.73562	2.08156	1.11291
C	5.16706	3.64408	-2.15102
H	3.19237	3.42518	-2.96495
C	5.98508	3.44581	-1.03491
H	6.10239	2.73224	0.99441
H	5.57294	4.08041	-3.05819
H	7.03192	3.72976	-1.074
H	0.14306	1.51709	-0.45566
O	-1.89652	1.52106	-0.62609
C	-2.63208	2.52937	-0.19779
O	-3.27565	2.51513	0.84853
C	-2.68695	3.74873	-1.15136
C	-1.32539	4.01148	-1.81854
H	-0.99382	3.13945	-2.38798
H	-1.40215	4.85945	-2.5072
H	-0.56118	4.26178	-1.07475
C	-3.14511	4.9936	-0.37327
H	-3.25453	5.8456	-1.05199
H	-4.10204	4.81648	0.12034
H	-2.42074	5.26695	0.40031
C	-3.72693	3.40124	-2.24419
H	-4.71103	3.21118	-1.80447
H	-3.82873	4.23776	-2.94369
H	-3.42133	2.51604	-2.81117

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Sum of electronic and thermal Free Energies: -2016.713227

C	2.46141900	-1.06381400	-2.72631500
C	2.47537700	-1.76642200	-3.93021200
H	2.69640400	-1.25074700	-4.85934200
C	2.18531800	-3.13118200	-3.91687800
C	1.88199000	-3.77361000	-2.71354000
H	1.66801500	-4.83815100	-2.70686600
C	1.87045200	-3.05466200	-1.51342600
C	2.15223000	-1.68500300	-1.50023500
H	1.66945800	-3.56821900	-0.57765400
C	-2.43949300	-2.65587100	0.49007600
C	-2.97534400	-2.35044000	-0.80455400
C	-4.08411700	-1.40540100	-0.63851300
C	-4.17568800	-1.08371800	0.74753900
C	-3.13680200	-1.83945900	1.44419400
Rh	-2.17485900	-0.50235500	0.00549600
H	2.19402600	-3.69174900	-4.84630200
C	-5.21055100	-0.22510500	1.39877500
H	-4.85323200	0.18227300	2.34698300

H	-6.10266000	-0.82831100	1.61151100
H	-5.48529500	0.60734600	0.75199400
C	-2.90748800	-1.82885500	2.91894300
H	-3.58012800	-2.55656900	3.39248300
H	-3.12165000	-0.85088900	3.35324000
H	-1.88259400	-2.10134500	3.17573200
C	-4.99170300	-0.92774200	-1.72236800
H	-5.27733600	0.11059500	-1.55370100
H	-5.89502900	-1.55170100	-1.73786100
H	-4.52136000	-1.00272900	-2.70480100
C	-2.53006300	-2.94441200	-2.10082700
H	-2.72661000	-2.27198700	-2.93811000
H	-3.07826200	-3.87702900	-2.28768000
H	-1.46274100	-3.17483400	-2.09161500
C	-1.35521200	-3.64113400	0.79579500
H	-0.74884400	-3.32170100	1.64604800
H	-0.69407300	-3.78570600	-0.06007800
H	-1.79626900	-4.61367900	1.04637700
N	2.78168900	0.30878600	-2.61415700
O	-0.07308900	-0.49035700	-0.33839300
C	2.23218000	-0.84151600	-0.25335300
C	0.96738600	-0.59638100	0.39762600
C	0.79833100	-0.41466400	1.87047500
C	1.34690900	-1.33083000	2.78319700
C	0.00708600	0.64387500	2.35030600
C	1.10204700	-1.19352700	4.14950300
H	1.96779800	-2.14429800	2.42336600
C	-0.20503900	0.79673300	3.72109400
H	-0.42009800	1.35339600	1.64856100
C	0.33611600	-0.12378400	4.62215000
H	1.52284400	-1.91186000	4.84647700
H	-0.78982500	1.63627900	4.08548100
H	0.16703000	-0.00616600	5.68832300
C	3.53060000	-0.87115400	0.48950800
C	4.51838300	-1.82986400	0.19063700
C	3.84302800	0.10355200	1.46061300
C	5.74053700	-1.84225300	0.86416100
H	4.32971800	-2.58030800	-0.56865000
C	5.06252300	0.08774900	2.13302800
H	3.12736300	0.88472900	1.68881300
C	6.01798400	-0.88878200	1.84358800
H	6.47694500	-2.60187100	0.61842400
H	5.27015900	0.84955800	2.87880100
H	6.96937500	-0.89860000	2.36661600
C	2.21948800	0.93039600	-1.53038800
H	1.13278500	0.87916200	-1.50618900
C	2.84179400	2.12444600	-0.96641100
C	2.01781500	3.09860900	-0.37127300
C	4.23392500	2.33243500	-0.99236800
C	2.56792100	4.26205700	0.15756100
H	0.94408600	2.93945700	-0.34608600
C	4.78036400	3.50045800	-0.46718700
H	4.89613500	1.57242000	-1.39685600
C	3.94999600	4.46759500	0.10536700
H	1.92163600	5.01245500	0.60207500
H	5.85465100	3.65276100	-0.49442000
H	4.37935000	5.37736200	0.51372600
H	2.54226823	0.77614694	-3.48094782
O	-2.01395200	1.47295100	-0.36584800
C	-3.04952300	2.26737800	-0.61118400
O	-4.21324400	1.88295600	-0.63985300
C	-2.66421400	3.73888400	-0.87394500
C	-1.73098100	3.79626800	-2.10325700
H	-0.82423500	3.20715300	-1.94684300
H	-1.44045500	4.83288100	-2.30354100
H	-2.23485900	3.41395000	-2.99750100
C	-3.93427600	4.56058000	-1.14515700
H	-3.66728700	5.60520800	-1.33597900
H	-4.61793900	4.52978300	-0.29280800
H	-4.47432800	4.17837300	-2.01497000
C	-1.93886500	4.29710500	0.36987100
H	-2.58777900	4.26883600	1.25213400
H	-1.65666200	5.34153900	0.20001400
H	-1.03263700	3.72892000	0.59653600

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Sum of electronic and thermal Free Energies: -2016.729656

C	2.93677600	-1.68842000	-2.17806800
C	3.21451100	-2.81078500	-2.96392600
H	3.52550500	-2.70156700	-3.99856000
C	3.08579200	-4.07558900	-2.38512200
C	2.69010200	-4.22578700	-1.05226900
H	2.60459700	-5.21653800	-0.61789200
C	2.41807100	-3.09410800	-0.27080000
C	2.53247100	-1.82744600	-0.83665800
H	2.12126800	-3.21866500	0.76602900
C	-2.34481000	-2.77749700	-0.13895700
C	-2.57671900	-2.26192100	-1.45179700
C	-3.75656100	-1.39277700	-1.40831100

C	-4.22111500	-1.35013600	-0.05451300
C	-3.32491800	-2.18191700	0.73741200
Rh	-2.17865100	-0.55150400	-0.14492800
H	3.29878000	-4.95580200	-2.98455000
C	-5.46813700	-0.68359200	0.42831700
H	-5.45864500	-0.54125700	1.51065600
H	-6.33134100	-1.31613700	0.18426000
H	-5.59421900	0.28947500	-0.04712500
C	-3.44864200	-2.43484600	2.20321400
H	-4.05431300	-3.33646200	2.36487800
H	-3.94447800	-1.60780600	2.71423100
H	-2.47598300	-2.59865000	2.67108100
C	-4.39942100	-0.71464900	-2.57066800
H	-4.63810600	0.31988600	-2.31250400
H	-5.33171200	-1.23562800	-2.82460000
H	-3.75900700	-0.72507700	-3.45409700
C	-1.78777300	-2.58449000	-2.67848900
H	-1.75688800	-1.73864900	-3.36889600
H	-2.25812900	-3.42417500	-3.20628600
H	-0.76275900	-2.87169100	-2.43728000
C	-1.28121300	-3.75121300	0.26118900
H	-1.00028100	-3.63151200	1.30957200
H	-0.37944700	-3.64518600	-0.34524900
H	-1.65152800	-4.77591200	0.13310800
N	3.03643600	-0.34811100	-2.51808400
O	-0.03148600	-0.28961700	-0.14111300
C	2.34734400	-0.42118800	-0.22901900
C	1.00643200	-0.41153900	0.53677900
C	0.89772100	-0.58743300	2.00646000
C	1.84005800	-1.30933600	2.76288700
C	-0.21460900	-0.01858000	2.66041900
C	1.64318900	-1.50105400	4.12878100
H	2.72504000	-1.71649000	2.29151200
C	-0.38559000	-0.18478800	4.03206100
H	-0.90555500	0.60193900	2.09857500
C	0.53492400	-0.93873900	4.76637600
H	2.36737600	-2.07396200	4.69896700
H	-1.22681900	0.28511900	4.53247500
H	0.39885100	-1.07160200	5.83544200
C	3.54831500	0.05236100	0.59979900
C	4.77595600	-0.62115000	0.55741100
C	3.45491600	1.22226500	1.37073200
C	5.87440300	-0.14868200	1.28023300
H	4.88006700	-1.52031200	-0.03935600
C	4.54840100	1.69128600	2.09566800
H	2.52397500	1.78031300	1.40139400
C	5.76407000	1.00509700	2.05500600
H	6.81649600	-0.68683200	1.23344500
H	4.45152500	2.59659700	2.68735000
H	6.61725000	1.37033900	2.61861200
C	2.19666200	0.42395300	-1.59328000
H	1.14247900	0.31974900	-1.87569900
C	2.52922600	1.89624700	-1.56299100
C	1.50673400	2.82071600	-1.30366700
C	3.82636800	2.36592600	-1.80393300
C	1.77991500	4.18856900	-1.26948300
H	0.49302700	2.46592600	-1.13048300
C	4.09619300	3.73475000	-1.78123700
H	4.61924000	1.65396200	-2.00814600
C	3.07627900	4.64891600	-1.51073300
H	0.97962900	4.89462300	-1.06800300
H	5.10511500	4.08729400	-1.97399400
H	3.28830400	5.71382200	-1.49497600
H	2.97598700	-0.09069700	-3.49514500
O	-2.16756200	1.43614400	0.11246700
C	-3.17620000	2.25237300	-0.16952900
O	-4.19442400	1.89227800	-0.75209300
C	-2.95550800	3.72686000	0.22814500
C	-2.56276900	4.47374600	-1.07009500
H	-1.62452300	4.09033200	-1.48556300
H	-2.42785700	5.53943300	-0.85768200
H	-3.34266300	4.37189700	-1.82979200
C	-4.28783300	4.29024400	0.76098300
H	-4.18202100	5.35893400	0.97268800
H	-4.58557000	3.79305900	1.69076400
H	-5.08852000	4.15511700	0.03138100
C	-1.85006000	3.89192600	1.28414700
H	-2.09388000	3.35364100	2.20628900
H	-1.74049400	4.95121900	1.53894700
H	-0.88548800	3.52647300	0.92364700

iso-p

Sum of electronic and thermal Free Energies: -1171.148602

C	-0.21668500	2.78865100	-0.37540200
C	0.10869600	4.14393300	-0.29753100
H	-0.65261900	4.90624600	-0.43742200
C	1.43785600	4.49414200	-0.04594100
C	2.41786400	3.51436300	0.12488800
H	3.44849100	3.80121900	0.30883200

C	2.07839800	2.15630100	0.05252400
C	0.75969900	1.78968100	-0.20058400
H	2.85094000	1.40668900	0.17879200
H	1.70934800	5.54481500	0.00840500
N	-1.47051900	2.22081400	-0.58876700
O	0.51774300	-0.77677500	-2.35592300
C	0.07533500	0.41340000	-0.30749900
C	0.89536300	-0.55265900	-1.21356600
C	2.17253000	-1.19912200	-0.74072000
C	2.68811800	-1.11438500	0.56391700
C	2.88610400	-1.94178000	-1.69925700
C	3.88619100	-1.74922600	0.89301200
H	2.15549900	-0.56628900	1.32994700
C	4.07987900	-2.57459800	-1.36903700
H	2.47955000	-2.00384600	-2.70232900
C	4.58444700	-2.48004800	-0.06904800
H	4.26933500	-1.67619500	1.90656100
H	4.61844500	-3.14085400	-2.12338400
H	5.51574000	-2.97460200	0.19248200
C	-0.25437200	-0.21320600	1.05663800
C	-0.25409800	0.54339400	2.23582500
C	-0.62435400	-1.56549000	1.13349200
C	-0.60007700	-0.03819900	3.45801300
H	0.02350500	1.59108800	2.20048700
C	-0.96528800	-2.14794300	2.35293800
H	-0.65277100	-2.16896700	0.23120700
C	-0.95261700	-1.38606000	3.52295600
H	-0.59164800	0.56752900	4.36004300
H	-1.24398500	-3.19729800	2.38696600
H	-1.21738100	-1.83859100	4.47434600
C	-1.25685800	0.84640600	-1.07677500
H	-0.97357400	0.86130700	-2.13600600
C	-2.48867400	-0.02227700	-0.93478900
C	-2.70870300	-1.06438100	-1.84716300
C	-3.43386400	0.20259300	0.07474700
C	-3.84207100	-1.87169700	-1.74387100
H	-1.98066500	-1.24001500	-2.63335700
C	-4.57022600	-0.60104000	0.17390500
H	-3.27040700	1.01308600	0.77712000
C	-4.77761700	-1.64207600	-0.73302100
H	-3.99818700	-2.67496600	-2.45881200
H	-5.29470400	-0.41326500	0.96173500
H	-5.66378000	-2.26602200	-0.65589600
H	-2.12930700	2.76537100	-1.13283400

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Sum of electronic and thermal Free Energies: -1591.207376

C	0.68806900	2.11574600	-0.17369200
C	1.08205400	3.39111800	-0.57849800
H	2.06906000	3.57768200	-0.98819100
C	0.16163000	4.43632400	-0.48528100
C	-1.12925100	4.20438300	-0.00296300
H	-1.83306300	5.02669600	0.07880400
C	-1.51370700	2.91368100	0.36337200
C	-0.61911000	1.83432100	0.27866700
H	-0.54325200	1.11961700	1.60136300
H	-2.51673900	2.74581400	0.74375100
C	-2.15370300	-2.24170800	0.19693900
C	-3.06971700	-1.12028700	0.43674200
C	-3.08619200	-0.29781400	-0.73129900
C	-2.08747400	-0.81679400	-1.64543800
C	-1.56755400	-2.06362900	-1.07686900
Rh	-1.04503300	-0.26002500	0.15109000
H	0.45595900	5.43300500	-0.79782500
C	-1.81828400	-0.32177800	-3.03158700
H	-0.79394300	-0.53741000	-3.34276400
H	-2.49250600	-0.81723500	-3.74213600
H	-1.98159000	0.75464200	-3.11423200
C	-0.55964800	-2.93945400	-1.75197300
H	-1.02690500	-3.47603800	-2.58630000
H	0.26523200	-2.34764300	-2.15866600
H	-0.14294500	-3.68058000	-1.06823200
C	-4.00211600	0.85306900	-1.00437000
H	-3.51589300	1.63101200	-1.59594300
H	-4.87007500	0.49669900	-1.57315300
H	-4.37922100	1.30301000	-0.08396800
C	-3.94019500	-0.98106200	1.64647300
H	-4.30268600	0.04090500	1.77198700
H	-4.81504700	-1.63693100	1.55352700
H	-3.40686000	-1.26342300	2.55656900
C	-1.91544900	-3.35602800	1.16620700
H	-1.02977300	-3.93874100	0.90857000
H	-1.78861000	-2.97807700	2.18396700
H	-2.77588000	-4.03665400	1.17159500
N	1.58435900	0.99054100	-0.20120100
O	1.00134100	-0.20543000	-0.34006800
C	2.88570900	1.10661000	-0.06248500
H	3.21868300	2.12793000	0.07641500
C	3.89518500	0.08130800	-0.06316100

C	5.22718400	0.53489100	0.09910300
C	3.65763300	-1.30663600	-0.20270300
C	6.28548900	-0.36228000	0.11821800
H	5.42090000	1.59833600	0.21014400
C	4.72664300	-2.19497700	-0.18001500
H	2.64457600	-1.66144500	-0.32048300
C	6.03653900	-1.73139100	-0.02175500
H	7.30085000	-0.00058100	0.24251700
H	4.54001900	-3.25900800	-0.28552500
H	6.86252900	-2.43581700	-0.00651500
Cl	-0.33764700	0.12937200	2.71369800

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Sum of electronic and thermal Free Energies: -1591.205726

C	1.34578	0.96086	-0.39863
C	2.25892	1.88778	-0.89906
H	3.13875	1.56945	-1.44631
C	2.01327	3.2448	-0.68198
C	0.87728	3.65595	0.022
H	0.70797	4.71256	0.20569
C	-0.04757	2.7108	0.47108
C	0.15065	1.33938	0.24818
H	0.00995	0.49642	1.52673
H	-0.93146	3.04418	1.00634
C	-3.28853	-1.32435	0.33241
C	-3.43057	0.08486	0.71834
C	-3.1713	0.88951	-0.43352
C	-2.72961	0.0036	-1.49541
C	-2.87566	-1.37459	-1.01937
Rh	-1.31795	-0.21959	0.10396
H	2.7131	3.98073	-1.06506
C	-2.40601	0.39471	-2.90279
H	-1.66707	-0.28069	-3.34007
H	-3.31092	0.34666	-3.52196
H	-2.01494	1.41243	-2.96009
C	-2.58319	-2.58877	-1.84456
H	-3.36346	-2.72716	-2.60258
H	-1.62584	-2.48797	-2.36466
H	-2.54266	-3.4929	-1.23485
C	-3.36897	2.36684	-0.55909
H	-2.63929	2.82187	-1.23192
H	-4.36708	2.56304	-0.97005
H	-3.31123	2.87104	0.40723
C	-3.92202	0.55518	2.05248
H	-3.67246	1.60309	2.2293
H	-5.01382	0.45843	2.10842
H	-3.4929	-0.03537	2.86512
C	-3.53921	-2.47602	1.25335
H	-3.13247	-3.40945	0.86072
H	-3.09908	-2.29979	2.23826
H	-4.61942	-2.61076	1.39401
N	1.50488	-0.45714	-0.59398
O	0.34311	-1.10491	-0.82546
C	2.59489	-1.18451	-0.58834
H	2.38325	-2.20786	-0.87916
C	3.96817	-0.86839	-0.24023
C	4.94259	-1.7554	-0.74721
C	4.37756	0.16452	0.63372
C	6.28844	-1.58619	-0.43805
H	4.63442	-2.57404	-1.38834
C	5.72244	0.31614	0.94935
H	3.64853	0.82873	1.08088
C	6.68235	-0.54799	0.40224
H	7.02651	-2.26981	-0.84878
H	6.02712	1.10614	1.63025
H	7.7311	-0.41727	0.65333
Cl	-0.138	-0.60549	2.51303

TS12(Ir)

Sum of electronic and thermal Free Energies: -1472.471487

C	-0.55908	-1.84653	1.43546
C	-0.70321	-3.10391	2.01401
H	-1.52692	-3.75709	1.7452
C	0.26249	-3.53108	2.93007
C	1.34888	-2.71124	3.25151
H	2.08037	-3.04523	3.98064
C	1.48629	-1.46672	2.63825
C	0.54557	-1.00602	1.69631
H	0.26527	0.18161	1.80779
H	2.31073	-0.81564	2.91286
C	2.71852	0.89926	-1.40926
C	3.23802	-0.08662	-0.49827
C	2.69979	-1.39184	-0.89139
C	1.82981	-1.18875	-2.00786
C	1.80345	0.23807	-2.31887
O	0.20589	1.87426	0.09813
C	-0.32074	2.20755	1.22768
O	-0.37279	1.44208	2.21863
C	-0.91276	3.62336	1.34297
H	0.16342	-4.50918	3.38993

C	1.0596	-2.23395	-2.752
H	0.03091	-1.91019	-2.93017
H	1.52823	-2.41984	-3.72567
H	1.02982	-3.17932	-2.2078
C	1.09262	0.87175	-3.47498
H	0.8264	1.9082	-3.25815
H	1.73455	0.86654	-4.36463
H	0.1761	0.33182	-3.72337
C	3.10158	-2.71152	-0.30762
H	2.31774	-3.46235	-0.42491
H	4.00027	-3.08218	-0.81513
H	3.32925	-2.63171	0.75635
C	4.29047	0.14708	0.54302
H	4.25326	-0.6083	1.32968
H	5.286	0.09748	0.08521
H	4.18632	1.12875	1.00993
C	3.03763	2.36039	-1.41555
H	3.78491	2.57122	-2.19033
H	2.14815	2.95738	-1.62813
H	3.44382	2.6879	-0.45652
N	-1.52021	-1.32998	0.49783
O	-1.02437	-0.57308	-0.48709
C	-0.19453	4.33897	2.50894
H	0.87321	4.4677	2.30001
H	-0.62824	5.33337	2.65418
H	-0.29812	3.77503	3.43858
C	-2.41372	3.46473	1.6777
H	-2.86828	4.45194	1.80757
H	-2.94939	2.95196	0.87093
H	-2.54914	2.89497	2.59999
C	-0.7423	4.42196	0.04228
H	-1.23696	3.92938	-0.79928
H	-1.1841	5.41624	0.16265
H	0.31302	4.5513	-0.21387
C	-2.81008	-1.5496	0.61312
H	-3.07405	-2.13678	1.48456
C	-3.8824	-1.10713	-0.24101
C	-5.1826	-1.51386	0.14493
C	-3.7313	-0.31049	-1.40067
C	-6.29315	-1.14352	-0.60059
H	-5.31052	-2.12286	1.03589
C	-4.85261	0.05397	-2.13837
H	-2.74454	0.01116	-1.69953
C	-6.1299	-0.35747	-1.74592
H	-7.28344	-1.46318	-0.293
H	-4.7315	0.6663	-3.0265
H	-6.99719	-0.06536	-2.33012
Ir	1.04876	-0.0105	-0.29338

TS89(Cl)

Sum of electronic and thermal Free Energies: -1591.205726

C	1.34578	0.96086	-0.39863
C	2.25892	1.88778	-0.89906
H	3.13875	1.56945	-1.44631
C	2.01327	3.2448	-0.68198
C	0.87728	3.65595	0.022
H	0.70797	4.71256	0.20569
C	-0.04757	2.7108	0.47108
C	0.15065	1.33938	0.24818
H	0.00995	0.49642	1.52673
H	-0.93146	3.04418	1.00634
C	-3.28853	-1.32435	0.33241
C	-3.43057	0.08486	0.71834
C	-3.1713	0.88951	-0.43352
C	-2.72961	0.0036	-1.49541
C	-2.87566	-1.37459	-1.01937
Rh	-1.31795	-0.21959	0.10396
H	2.7131	3.98073	-1.06506
C	-2.40601	0.39471	-2.90279
H	-1.66707	-0.28069	-3.34007
H	-3.31092	0.34666	-3.52196
H	-2.01494	1.41243	-2.96009
C	-2.58319	-2.58877	-1.84456
H	-3.36346	-2.72716	-2.60258
H	-1.62584	-2.48797	-2.36466
H	-2.54266	-3.4929	-1.23485
C	-3.36897	2.36684	-0.55909
H	-2.63929	2.82187	-1.23192
H	-4.36708	2.56304	-0.97005
H	-3.31123	2.87104	0.40723
C	-3.92202	0.55518	2.05248
H	-3.67246	1.60309	2.2293
H	-5.01382	0.45843	2.10842
H	-3.4929	-0.03537	2.86512
C	-3.53921	-2.47602	1.25335
H	-3.13247	-3.40945	0.86072
H	-3.09908	-2.29979	2.23826
H	-4.61942	-2.61076	1.39401
N	1.50488	-0.45714	-0.59398

O	0.34311	-1.10491	-0.82546
C	2.59489	-1.18451	-0.58834
H	2.38325	-2.20786	-0.87916
C	3.96817	-0.86839	-0.24023
C	4.94259	-1.7554	-0.74721
C	4.37756	0.16452	0.63372
C	6.28844	-1.58619	-0.43805
H	4.63442	-2.57404	-1.38834
C	5.72244	0.31614	0.94935
H	3.64853	0.82873	1.08088
C	6.68235	-0.54799	0.40224
H	7.02651	-2.26981	-0.84878
H	6.02712	1.10614	1.63025
H	7.7311	-0.41727	0.65333
Cl	-0.138	-0.60549	2.51303