SUPPLEMENTARY INFORMATION

Mechanistic Insight into the Highly Regioselective Ni(0)-Catalyzed [2+2] Self-cycloaddition of Electron-Deficient Allenoates

Dandan Jiang[a], Qianqian Li[a], Mingxing Fu[a], Xuefei Zhao[a], Qingyong Meng[b], Lili Zhao*[a]

[a]*Institute of Advanced Synthesis, School of Chemistry and Molecular Engineering, Jiangsu National Synergetic Innovation Center for Advanced Materials, Nanjing Tech University, Nanjing 211816, China*

[b]*School of Natural and Applied Science, Northwestern Polytechnical University, 710000, Xi'an, China.*

Table of Contents

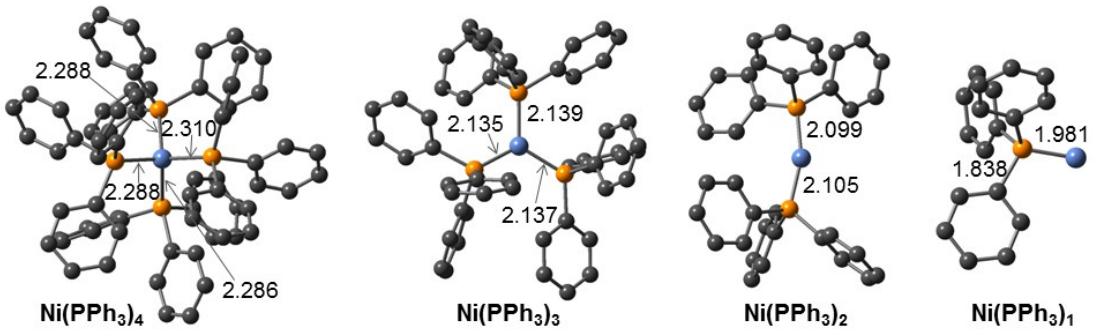

Fig. S1 Optimized geometries of $Ni(PPh_3)_x$ (x = 1-4). The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, P: orange, Ni: gray blue).

$Ni(PPh_3)_4 \longrightarrow Ni(PPh_3)_3 + PPh_3$ ($\Delta G[\Delta H]$ = -49.4[-27.2])

$Ni(PPh_3)_4 \longrightarrow Ni(PPh_3)_2 + 2\ PPh_3$ ($\Delta G[\Delta H]$ = -51.0[-13.0])

$Ni(PPh_3)_4 \longrightarrow Ni(PPh_3)_1 + 3\ PPh_3$ ($\Delta G[\Delta H]$ = -32.5[17.6])

$Ni(cod)_2 + 2\ PPh_3 \longrightarrow Ni(PPh_3)_2 + 2\ cod$ ($\Delta G[\Delta H]$ = 9.1[13.2])

Fig. S2 The calculated energetic results (in kcal mol^{-1}) for the decomposition of $Ni(PPh_3)_4$, and the ligand exchange reaction between the $Ni(cod)_2$ and $Ni(PPh_3)_2$.

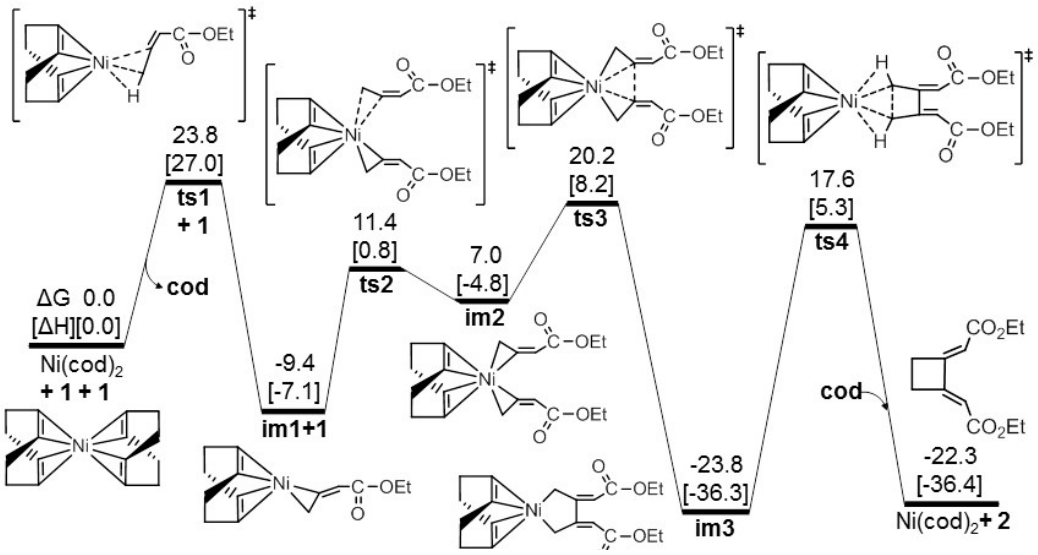

Fig. S3 Free energy profile for the $Ni(cod)_2$-mediated cyclodimerization of allenoates; enthalpies (in kcal mol^{-1}) are given in the brackets for reference. Optimized structures according to the energy profile are given in Fig. S4.

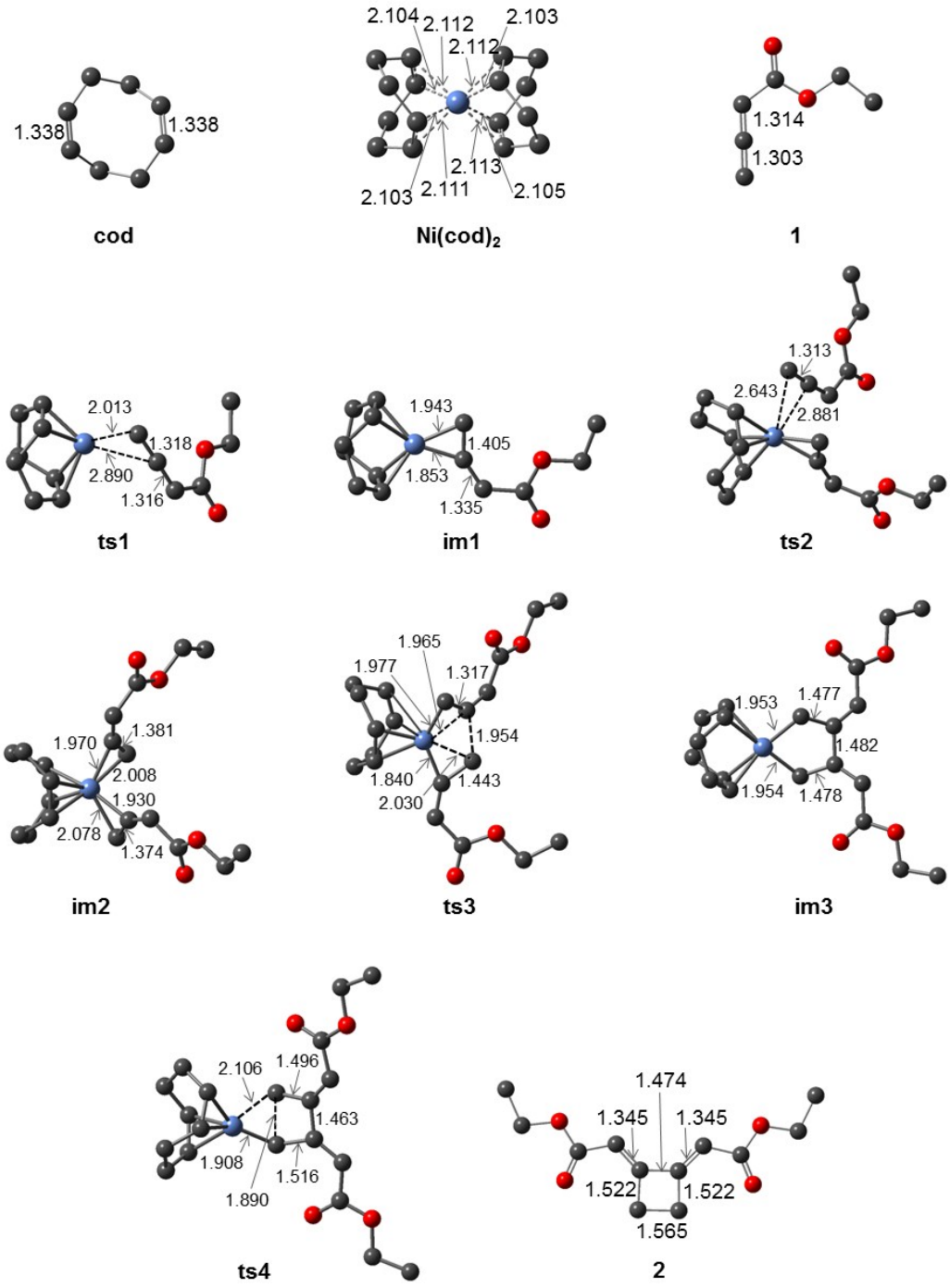

Fig. S4 Optimized geometries of $Ni(cod)_2$-mediated cyclodimerization of allenoates. The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, Ni: gray blue).

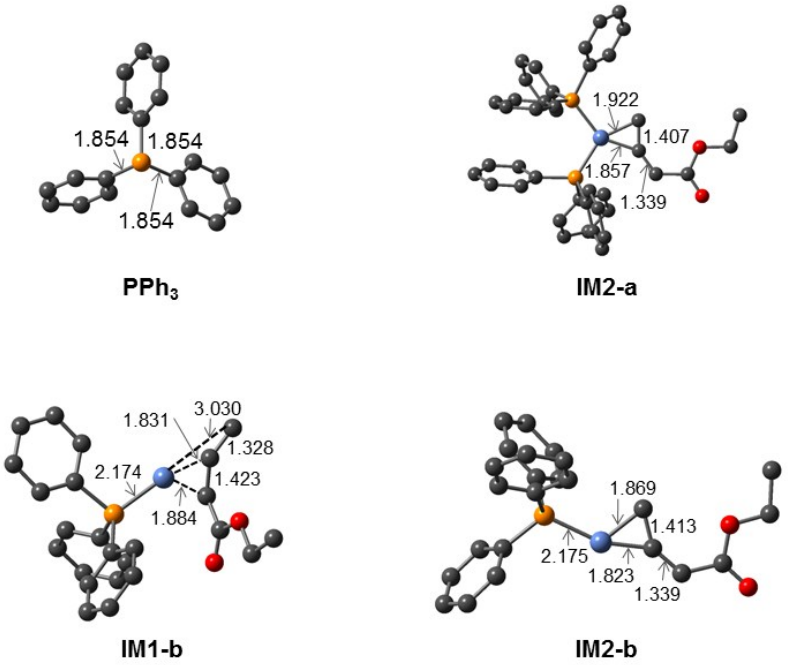

Fig. S5 Optimized structures according to the energy profile in Fig. 1. The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, P: orange, Ni: gray blue).

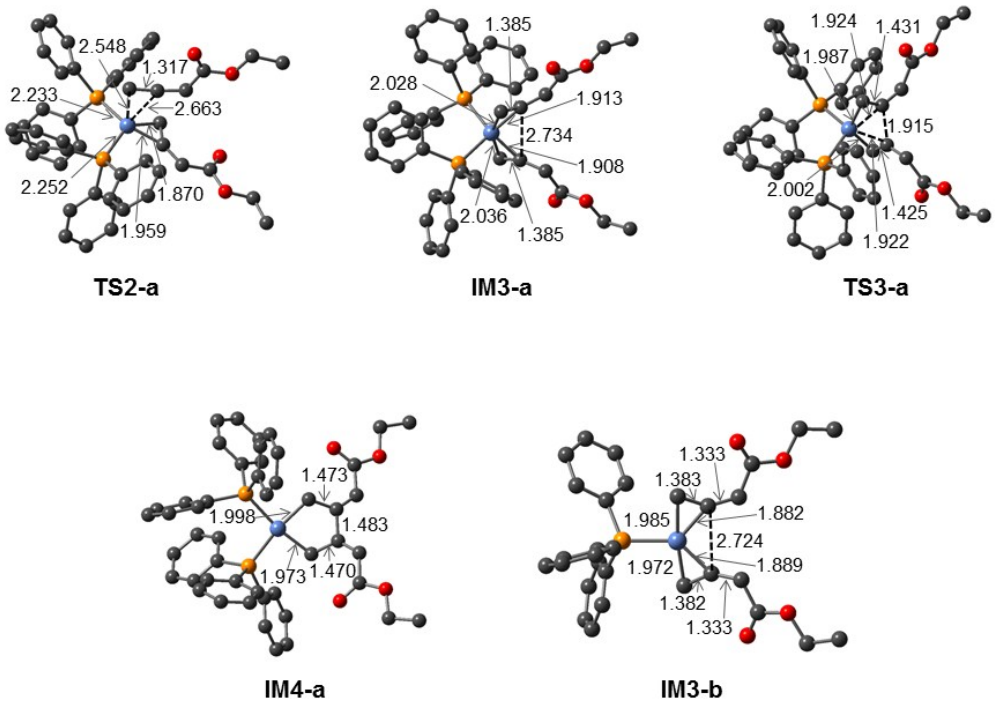

Fig. S6 Optimized structures according to the energy profile in Fig. 2. The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, P: orange, Ni: gray blue).

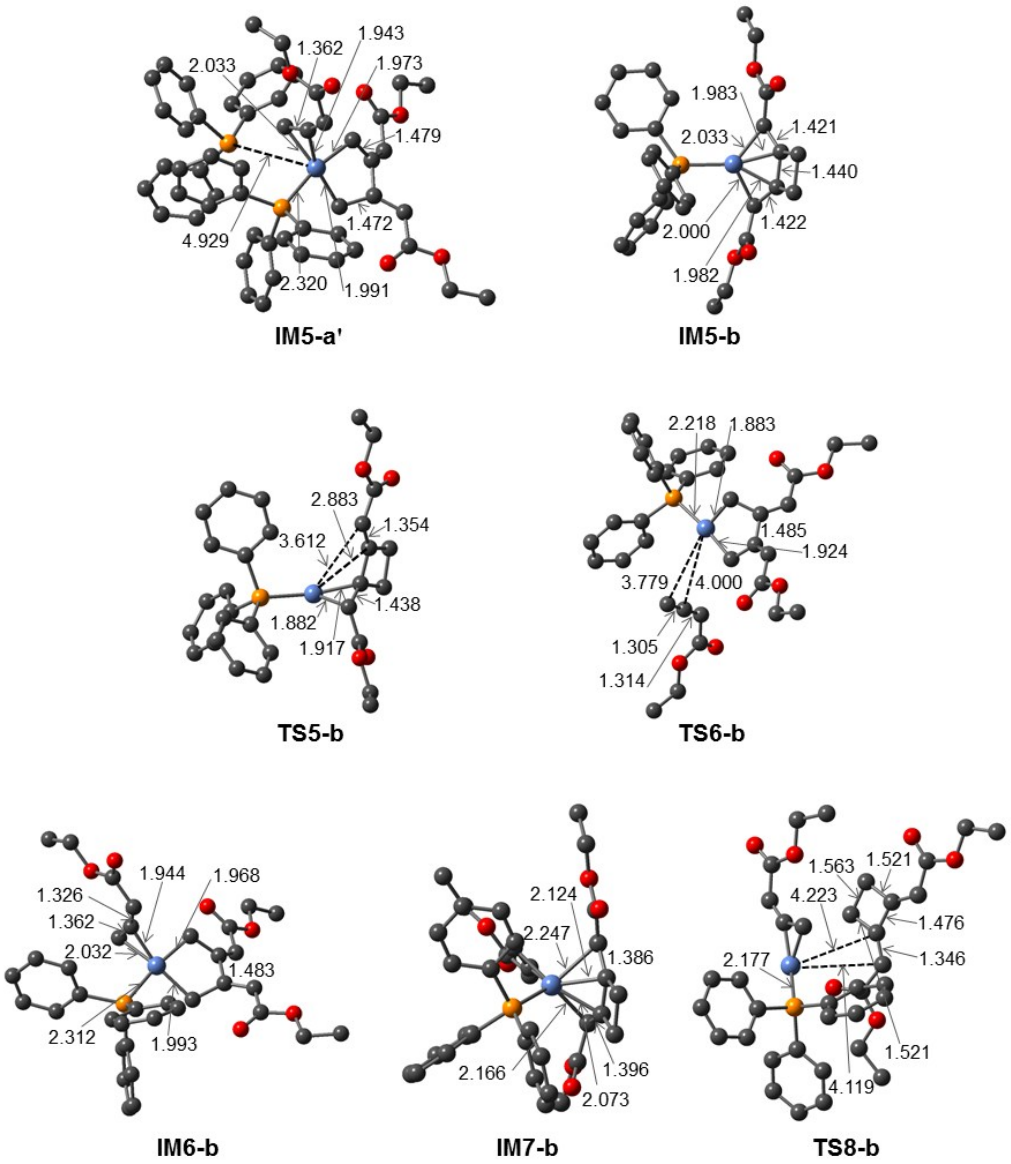

Fig. S7 Optimized structures according to the energy profile in Fig. 3. The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, P: orange, Ni: gray blue).

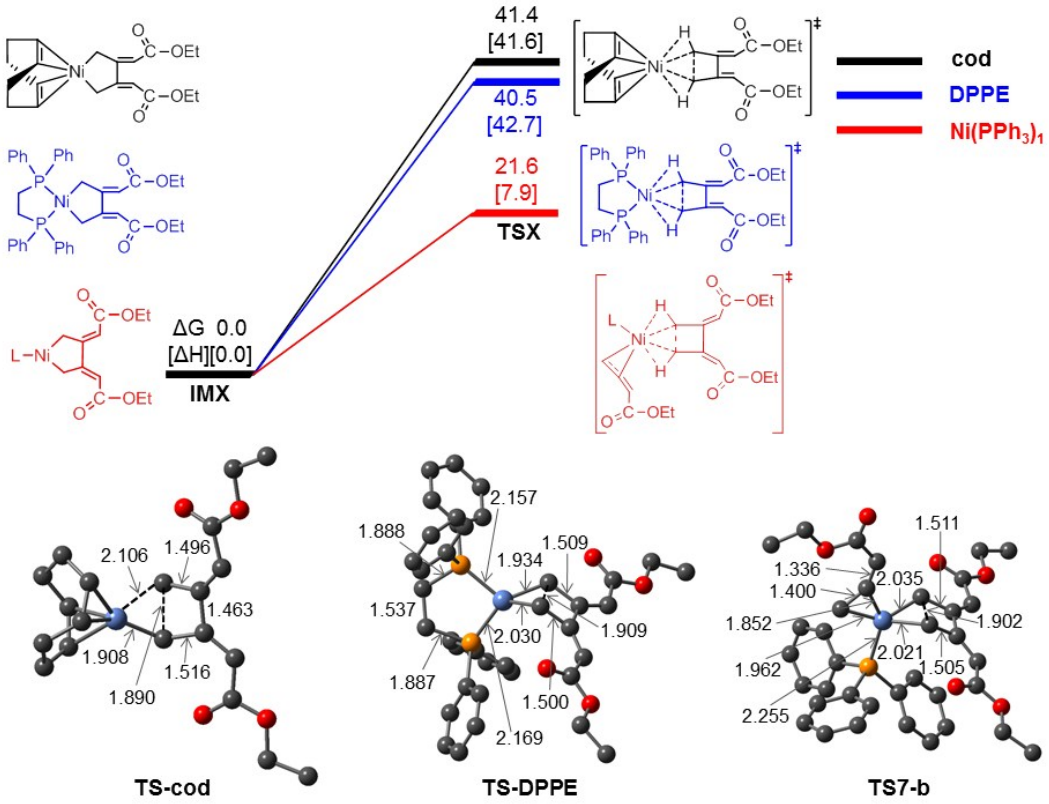

Fig. S8 Free energy profile (ΔG, in kcal mol^{-1}) and the optimized structures of the key transition states for the rate-determining step by using the different ligands.

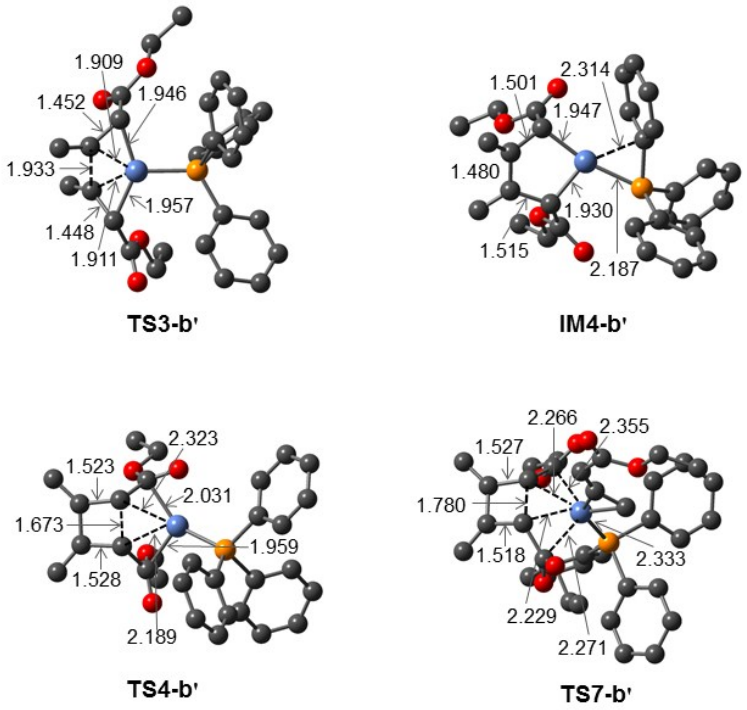

Fig. S9 Optimized structures for the rate-determining step for leading to different products. The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, P: orange, Ni: gray blue).

Table S1. Coordinates and energies (in hatree) of the calculated structures at the B3LYP/6-311++G(2d,p)-SOL//B3LYP/6-31G(d) level .

1

Free Energy = -383.889602848

Energy = -383.983336848

C	0.095684	1.011219	-0.000035
O	-0.444127	2.099713	-0.000072
O	-0.570028	-0.163306	-0.000002
C	-2.011587	-0.063896	-0.000021
H	-2.327199	0.501479	-0.883018
H	-2.327218	0.501544	0.882927
C	-2.564281	-1.476746	0.000025
H	-3.659371	-1.447063	0.000012
H	-2.233911	-2.026063	-0.887393
H	-2.233930	-2.025997	0.887492
C	1.571086	0.838455	-0.000005
C	2.189275	-0.320751	0.000034
C	2.818148	-1.462036	0.000073
H	3.087125	-1.961728	-0.928366
H	3.087098	-1.961681	0.928545
H	2.130696	1.770788	-0.000032

NiL_4

Free Energy = -5653.404551810

Energy = -5654.40395181

Ni	0.000075	0.021851	0.003418
P	1.427151	-1.712502	0.437438
P	0.897997	1.173950	-1.754547
P	-0.297540	1.559259	1.671653
P	-2.045033	-0.990335	-0.354250
C	2.474541	-2.363151	-0.974874
C	3.755714	-2.911566	-0.795338
C	1.937017	-2.369795	-2.266825
C	4.473006	-3.428653	-1.875270
H	4.203276	-2.937431	0.191705
C	2.644571	-2.895247	-3.350391
H	0.962826	-1.933931	-2.433271
C	3.921004	-3.424071	-3.158153
H	5.465739	-3.840488	-1.710398
H	2.199761	-2.872812	-4.341777
H	4.481150	-3.827842	-3.997773
C	2.815477	-1.492311	1.681059
C	3.036965	-2.318161	2.794477
C	3.730637	-0.453703	1.441140
C	4.120672	-2.096623	3.649884
H	2.371766	-3.148781	3.000553
C	4.824428	-0.245980	2.281408
H	3.594865	0.191275	0.581091
C	5.020821	-1.062470	3.397263
H	4.265087	-2.748547	4.508143
H	5.521478	0.557315	2.057392
H	5.868453	-0.897829	4.057487
C	0.737800	-3.348791	1.046587
C	0.977772	-4.570785	0.399792
C	-0.012247	-3.381145	2.234087
C	0.499276	-5.772480	0.926710
H	1.543111	-4.596608	-0.523615
C	-0.481526	-4.580469	2.769890
H	-0.223095	-2.462540	2.765954
C	-0.224433	-5.786761	2.118003
H	0.700428	-6.701665	0.399474
H	-1.050671	-4.566592	3.696099
H	-0.587917	-6.724320	2.530879
C	2.727655	1.462303	-1.572143
C	3.686873	0.624194	-2.167987
C	3.190078	2.486635	-0.728421
C	5.051740	0.827354	-1.957745
H	3.375669	-0.198392	-2.798826
C	4.555550	2.697736	-0.526785
H	2.480224	3.122084	-0.213642
C	5.494963	1.872134	-1.145766
H	5.766666	0.159575	-2.431227
H	4.875509	3.505107	0.125723
H	6.558424	2.035504	-0.990885
C	0.775711	0.569926	-3.533708
C	-0.377404	-0.129871	-3.907169
C	1.687231	0.917143	-4.543955
C	-0.602167	-0.512536	-5.231394
H	-1.126620	-0.349384	-3.156008
C	1.475405	0.525345	-5.866449
H	2.568582	1.503319	-4.307424
C	0.333545	-0.198429	-6.216534
H	-1.513315	-1.047247	-5.487520
H	2.201783	0.798527	-6.628044
H	0.168477	-0.498035	-7.248256
C	0.268842	2.883029	-2.240275
C	-1.093687	2.951831	-2.572249
C	1.047120	4.034079	-2.430353
C	-1.663267	4.123914	-3.065376
H	-1.718761	2.074220	-2.451427
C	0.473511	5.218080	-2.904467
H	2.111164	4.020214	-2.229026
C	-0.881950	5.270280	-3.225697
H	-2.719488	4.135762	-3.322109
H	1.099826	6.097225	-3.035641
H	-1.321899	6.188805	-3.605748
C	-2.069346	-2.783269	-0.907379
C	-2.679162	-3.803956	-0.161764
C	-1.476384	-3.140083	-2.129786
C	-2.705254	-5.120318	-0.627016
H	-3.138312	-3.580388	0.793013
C	-1.509294	-4.452092	-2.602627
H	-0.999442	-2.383549	-2.739294
C	-2.128266	-5.451511	-1.851963
H	-3.182007	-5.888054	-0.023069
H	-1.048417	-4.688895	-3.558388
H	-2.155763	-6.475625	-2.215193
C	-3.267745	-0.262490	-1.580208
C	-3.746342	1.031069	-1.311078
C	-3.768514	-0.923364	-2.712720
C	-4.679933	1.645008	-2.145533
H	-3.397862	1.558360	-0.431370
C	-4.691759	-0.301965	-3.559622
H	-3.454111	-1.935687	-2.939107

C	-5.151970	0.984025	-3.281756
H	-5.037352	2.641460	-1.899610
H	-5.059906	-0.837152	-4.431664
H	-5.875604	1.462596	-3.936547
C	-3.233305	-1.126898	1.089530
C	-4.621070	-1.274992	0.919533
C	-2.728394	-1.155640	2.392712
C	-5.465067	-1.434447	2.018775
H	-5.049551	-1.266668	-0.076918
C	-3.566317	-1.322374	3.498474
H	-1.668198	-1.016659	2.549507
C	-4.941403	-1.460359	3.314026
H	-6.535592	-1.541520	1.861650
H	-3.138548	-1.329573	4.497762
H	-5.601089	-1.585013	4.169059
C	-0.344739	1.092591	3.495041
C	-0.882281	1.932333	4.485365
C	0.314954	-0.068748	3.909014
C	-0.805731	1.588501	5.834659
H	-1.359457	2.866072	4.206506
C	0.406971	-0.412567	5.260404
H	0.791524	-0.694600	3.164884
C	-0.166336	0.409951	6.228661
H	-1.237132	2.249970	6.582004
H	0.936038	-1.317263	5.548544
H	-0.103055	0.146801	7.281405
C	0.977278	2.914952	1.989520
C	0.774319	4.299452	1.901686
C	2.224404	2.466372	2.455700
C	1.791620	5.198376	2.240693
H	-0.180752	4.701094	1.588443
C	3.232475	3.359059	2.810528
H	2.408441	1.402757	2.554200
C	3.024416	4.735710	2.697002
H	1.605307	6.266514	2.158803
H	4.181088	2.973730	3.175876
H	3.808382	5.437099	2.971142
C	-1.874369	2.536540	1.506704
C	-3.030288	2.247622	2.253072
C	-1.962965	3.549370	0.536591
C	-4.211359	2.966817	2.061084
H	-3.019923	1.454737	2.989817
C	-3.138013	4.280795	0.354766
H	-1.112863	3.763134	-0.098411
C	-4.269002	3.996965	1.121361
H	-5.088098	2.716174	2.652675
H	-3.163647	5.063479	-0.398537
H	-5.185745	4.564240	0.982278

NiL_3

Free Energy **=** -4617.188140810

Energy = -4617.91981281

Ni	-0.039800	0.055577	-0.121340
P	1.886751	0.981375	-0.129256
P	-1.863520	1.167481	-0.012484
P	-0.072143	-2.077022	-0.025381
C	2.277873	2.015436	-1.621734
C	1.211282	2.471677	-2.410712
C	3.585459	2.360807	-2.004070
C	1.439509	3.251527	-3.545945
H	0.196566	2.218124	-2.120713
C	3.815494	3.141025	-3.137738
H	4.429608	2.008899	-1.418889
C	2.742679	3.587853	-3.912732
H	0.597495	3.595672	-4.140883
H	4.834321	3.397692	-3.417223
H	2.923141	4.192801	-4.797692
C	3.437600	-0.053341	-0.043314
C	4.260184	-0.126976	1.088822
C	3.774404	-0.841660	-1.157622
C	5.381724	-0.961024	1.107249
H	4.033511	0.468855	1.966314
C	4.895816	-1.668524	-1.143650
H	3.156702	-0.804729	-2.049366
C	5.706872	-1.732262	-0.007340
H	6.004589	-0.999422	1.997643
H	5.136722	-2.262567	-2.021838
H	6.583132	-2.375487	0.005929
C	2.164132	2.126894	1.305759
C	2.742464	3.400232	1.196915
C	1.734584	1.693646	2.572899
C	2.881368	4.218943	2.320755
H	3.080530	3.761543	0.230858
C	1.885803	2.506069	3.696596
H	1.277067	0.712831	2.679344
C	2.456727	3.774842	3.573342
H	3.327180	5.204985	2.214552
H	1.549479	2.150152	4.666959
H	2.566249	4.412852	4.446422
C	-1.948189	3.004681	-0.332833
C	-3.008086	3.630351	-1.007842
C	-0.898485	3.807949	0.140722
C	-3.010915	5.012122	-1.211481
H	-3.837654	3.039791	-1.381889
C	-0.907360	5.190223	-0.047683
H	-0.061903	3.347593	0.655961
C	-1.962805	5.797592	-0.730339
H	-3.838736	5.474222	-1.743939
H	-0.082376	5.787667	0.331697
H	-1.966952	6.873073	-0.888551
C	-2.593604	1.046087	1.688315
C	-2.939079	-0.227579	2.176456
C	-2.748778	2.149752	2.539531
C	-3.430110	-0.389363	3.471830
H	-2.835167	-1.095374	1.533376
C	-3.228262	1.984161	3.841339
H	-2.495439	3.144880	2.190614
C	-3.571656	0.717254	4.312683
H	-3.699499	-1.382850	3.821319
H	-3.338187	2.853439	4.485048
H	-3.948202	0.592329	5.324694
C	-3.228582	0.598274	-1.133644
C	-4.543213	0.339995	-0.723222
C	-2.907784	0.426763	-2.491635
C	-5.505577	-0.092117	-1.640542
H	-4.821198	0.470847	0.317707
C	-3.867969	0.003930	-3.409420
H	-1.892189	0.618143	-2.831375
C	-5.172982	-0.261858	-2.984567

H	-6.518738	-0.291911	-1.300421
H	-3.597747	-0.122074	-4.454797
H	-5.922608	-0.596869	-3.696713
C	0.984960	-2.669476	1.370188
C	0.600737	-2.296526	2.672626
C	2.186721	-3.369994	1.204100
C	1.385319	-2.635743	3.774125
H	-0.323737	-1.743271	2.824509
C	2.975948	-3.701224	2.308348
H	2.520121	-3.649302	0.210578
C	2.577869	-3.341757	3.595445
H	1.065719	-2.346688	4.772356
H	3.907752	-4.239585	2.156175
H	3.192874	-3.602845	4.452737
C	0.537922	-2.954483	-1.540696
C	0.847120	-2.189052	-2.673102
C	0.636926	-4.352234	-1.630094
C	1.252678	-2.797420	-3.863252
H	0.765320	-1.106367	-2.612672
C	1.053941	-4.962827	-2.812728
H	0.375875	-4.967853	-0.773659
C	1.362034	-4.186357	-3.933053
H	1.481450	-2.185791	-4.732323
H	1.129530	-6.046132	-2.863410
H	1.678951	-4.663782	-4.856763
C	-1.627520	-3.080396	0.232602
C	-1.839730	-3.987470	1.281275
C	-2.650847	-2.914070	-0.716721
C	-3.043011	-4.692383	1.386211
H	-1.066168	-4.153385	2.023390
C	-3.846822	-3.622412	-0.617632
H	-2.515181	-2.216263	-1.537699
C	-4.050099	-4.513878	0.438799
H	-3.185515	-5.388123	2.209803
H	-4.622240	-3.470285	-1.363647
H	-4.984476	-5.063182	0.521266

NiL_2

Free Energy **=** -3580.895418040

Energy = -3581.37210604

P	2.091597	-0.002190	-0.233869
P	-2.056191	-0.025024	-0.252664
Ni	0.016076	-0.019699	-0.584284
C	2.579238	-1.423327	0.841638
C	1.543017	-2.317461	1.144052
C	1.772095	-3.433229	1.948564
C	3.049605	-3.663263	2.461574
C	4.090478	-2.776512	2.168566
C	3.859284	-1.661621	1.362017
H	0.562128	-2.082184	0.734675
H	0.957101	-4.115327	2.175770
H	3.236885	-4.529929	3.090460
H	5.084770	-2.955481	2.570006
H	4.677082	-0.981729	1.140751
C	2.642352	1.501519	0.684896
C	1.616655	2.267209	1.258063
C	1.909150	3.402580	2.012907
C	3.237968	3.788804	2.197169
C	4.267657	3.041833	1.618345
C	3.973549	1.904783	0.864488
H	0.592522	1.946149	1.076905
H	1.102649	3.986822	2.448072
H	3.472588	4.674252	2.782425
H	5.302163	3.348311	1.751527
H	4.780946	1.345965	0.399306
C	-3.159924	-1.193357	-1.170358
C	-2.594479	-2.398115	-1.616330
C	-3.369624	-3.349244	-2.279919
C	-4.724038	-3.105894	-2.515535
C	-5.297059	-1.907715	-2.085288
C	-4.521531	-0.958737	-1.416725
H	-1.534916	-2.579469	-1.449060
H	-2.914005	-4.275552	-2.620150
H	-5.328380	-3.842748	-3.038226
H	-6.349640	-1.709395	-2.271507
H	-4.975789	-0.024375	-1.099600
C	-2.394334	-0.415608	1.518128
C	-3.644225	-0.706778	2.080792
C	-3.746414	-0.964606	3.449056
C	-2.608392	-0.934209	4.261389
C	-1.359050	-0.652267	3.704789
C	-1.259023	-0.398355	2.338156
H	-4.533195	-0.741602	1.456914
H	-4.716377	-1.192589	3.883898
H	-2.697611	-1.137384	5.325599
H	-0.468585	-0.638319	4.327609
H	-0.316024	-0.199421	1.832263
C	-2.875232	1.611457	-0.515660
C	-3.211381	2.467145	0.542586
C	-3.725236	3.741491	0.289497
C	-3.909864	4.178939	-1.021920
C	-3.573347	3.335581	-2.084470
C	-3.055784	2.066427	-1.833478
H	-3.074988	2.138733	1.568287
H	-3.983275	4.391343	1.122016
H	-4.309911	5.170451	-1.216920
H	-3.711057	3.668683	-3.110009
H	-2.791459	1.419168	-2.666350
C	3.272660	-0.094202	-1.652857
C	3.523516	1.062674	-2.409457
C	4.308493	1.004717	-3.560014
C	4.848985	-0.212820	-3.981043
C	4.596745	-1.369834	-3.243121
C	3.813678	-1.312654	-2.088420
H	3.103329	2.013789	-2.092917
H	4.497242	1.911209	-4.129625
H	5.459800	-0.258669	-4.878798
H	5.011561	-2.322079	-3.564213
H	3.626123	-2.220950	-1.523624

NiL_1

Free Energy **=** -2544.570876210

Energy = -2544.79834621

Ni	-0.026012	-0.529548	2.435537
P	0.007451	-0.057516	0.512130
C	-0.063771	1.712190	0.024533
C	1.110556	2.480875	0.014213
C	-1.291079	2.344341	-0.221717

C	1.058705	3.849109	-0.249754
H	2.067292	2.005598	0.211995
C	-1.341031	3.713653	-0.485271
H	-2.209237	1.764516	-0.209960
C	-0.167245	4.469187	-0.501561
H	1.976150	4.432058	-0.259091
H	-2.298409	4.190666	-0.678987
H	-0.207277	5.535623	-0.707209
C	-1.434244	-0.832002	-0.330052
C	-1.661393	-0.932971	-1.708840
C	-2.380539	-1.360009	0.560506
C	-2.818548	-1.555203	-2.180311
H	-0.942399	-0.532348	-2.417693
C	-3.540427	-1.972918	0.092018
H	-2.140064	-1.262433	1.619422
C	-3.758201	-2.072827	-1.283688
H	-2.989803	-1.635730	-3.250762
H	-4.265929	-2.375403	0.793993
H	-4.657146	-2.554452	-1.659783
C	1.535706	-0.694448	-0.286032
C	2.343158	-1.458488	0.568438
C	1.940094	-0.495908	-1.613406
C	3.524413	-2.036505	0.109448
H	1.990174	-1.550087	1.595467
C	3.122231	-1.076591	-2.076200
H	1.350138	0.125293	-2.282167
C	3.911399	-1.849591	-1.219331
H	4.141193	-2.624840	0.783629
H	3.432271	-0.922194	-3.106590
H	4.830933	-2.297546	-1.587194

L= PPh_3

Free Energy **=** -1036.295169040

Energy = -1036.52285704

P	0.002362	-0.000447	-1.206321
C	-1.014518	-1.325936	-0.402034
C	-1.038295	-2.580178	-1.035053
C	-1.775936	-1.148981	0.763340
C	-1.784871	-3.633914	-0.508260
H	-0.470220	-2.728977	-1.950614
C	-2.532705	-2.200561	1.284807
H	-1.780942	-0.185069	1.263223
C	-2.536677	-3.445368	0.653389
H	-1.788139	-4.598082	-1.010155
H	-3.119328	-2.045727	2.186942
H	-3.127257	-4.262122	1.060130
C	-0.639909	1.542228	-0.402954
C	-0.101089	2.123595	0.754761
C	-1.725364	2.177498	-1.029750
C	-0.640247	3.302131	1.275478
H	0.744600	1.656405	1.250341
C	-2.271586	3.347768	-0.503414
H	-2.141872	1.752467	-1.940254
C	-1.727850	3.914774	0.651180
H	-0.209090	3.740742	2.171959
H	-3.113789	3.822386	-1.000353
H	-2.145306	4.832186	1.057839
C	1.659275	-0.216922	-0.403237
C	2.753869	0.402875	-1.029751
C	1.892049	-0.975621	0.754132
C	4.040281	0.287082	-0.503492
H	2.595813	0.976769	-1.940139
C	3.181883	-1.101343	1.274828
H	1.064280	-1.474308	1.249323
C	4.257823	-0.468178	0.650802
H	4.873614	0.777242	-1.000323
H	3.344532	-1.695049	2.170941
H	5.260865	-0.567861	1.057327

cod

Free Energy **=** -311.972469966

Energy = -312.121360966

C	1.735919	-0.669677	-0.119009
C	0.657284	-1.582688	0.422036
C	-0.657283	1.582692	-0.422033
C	-0.658709	-1.582101	-0.421977
C	-1.735922	0.669678	0.118998
C	-1.736683	-0.668184	0.118846
H	0.408701	-1.313019	1.457129
H	-0.409656	-1.312411	-1.456970
H	-0.408698	1.313034	-1.457129
H	1.054410	-2.603603	0.456685
H	-1.054407	2.603609	-0.456672
H	-1.056845	-2.602619	-0.457066
C	1.736681	0.668184	-0.118852
C	0.658708	1.582096	0.421981
H	0.409653	1.312392	1.456970
H	1.056847	2.602612	0.457086
H	2.587119	-1.169643	-0.581654
H	2.588052	1.167299	-0.582047
H	-2.588032	-1.167295	0.582085
H	-2.587120	1.169643	0.581647

Ni(cod)$_2$

Free Energy **=** -2132.264457060

Energy = -2132.58962706

C	2.229993	1.858463	0.527376
C	2.604633	0.633105	1.389788
C	1.329000	-1.500717	0.638214
C	1.474686	-0.389621	1.461523
H	1.699478	2.586242	1.154875
H	3.517152	0.161704	1.010503
H	3.138983	2.374146	0.176210
H	2.846502	0.966600	2.406074
H	0.978537	-0.444634	2.426986
H	0.753331	-2.333230	1.040235
C	2.227278	-1.859684	-0.528319
C	2.601964	-0.634653	-1.391280
C	1.329378	1.500475	-0.637707
C	1.472932	0.389345	-1.461553
H	1.694889	-2.586800	-1.154992
H	3.515554	-0.164342	-1.013193
H	3.136315	-2.376405	-0.178800
H	2.842128	-0.968483	-2.407860
H	0.976763	0.445444	-2.426936
H	0.754708	2.334023	-1.039043

Ni	0.000138	0.000831	0.000476
C	-2.228851	-1.859042	0.527682
C	-2.603409	-0.634035	1.390695
C	-1.329451	1.500618	0.638433
C	-1.473867	0.389187	1.461711
H	-1.697413	-2.586640	1.154591
H	-3.516503	-0.163069	1.012273
H	-3.137865	-2.375106	0.177154
H	-2.844290	-0.967984	2.407065
H	-0.977668	0.444872	2.427130
H	-0.754552	2.333731	1.040315
C	-2.228443	1.859158	-0.527741
C	-2.603216	0.634112	-1.390518
C	-1.329395	-1.500407	-0.638065
C	-1.473930	-0.389408	-1.461627
H	-1.696526	2.586398	-1.154684
H	-3.516322	0.163342	-1.011868
H	-3.137443	2.375722	-0.177855
H	-2.844237	0.967921	-2.406908
H	-0.977383	-0.444818	-2.426828
H	-0.753818	-2.333288	-1.039447

IM1-b

Free Energy **=** -2928.503035440

Energy = -2928.84462444

C	2.872261	-0.308320	1.012956
O	2.744119	0.690674	1.707226
O	3.731865	-0.354063	-0.035314
C	4.460343	0.860974	-0.300724
H	5.010198	1.152638	0.599989
H	3.747695	1.662910	-0.523543
C	5.390950	0.585940	-1.467930
H	5.971454	1.484999	-1.703869
H	6.088308	-0.222688	-1.227034
H	4.826388	0.294616	-2.359884
C	2.101547	-1.555001	1.204232
C	2.148166	-2.676389	0.330040
C	2.797630	-3.804620	0.068109
H	1.717230	-1.652795	2.221757
Ni	0.748690	-1.579284	-0.106591
P	-0.762208	-0.017393	-0.052631
C	-1.458048	0.338766	1.608412
C	-2.805882	0.131997	1.932577
C	-0.572470	0.800301	2.599464
C	-3.266166	0.389816	3.225874
H	-3.498474	-0.232227	1.180131
C	-1.041457	1.059670	3.886526
H	0.482861	0.941753	2.374100
C	-2.387030	0.855971	4.203333
H	-4.313164	0.224612	3.466616
H	-0.349956	1.415710	4.645457
H	-2.746737	1.054427	5.209562
C	-2.157637	-0.682840	-1.048089
C	-3.150046	0.066476	-1.693175
C	-2.154172	-2.080252	-1.191699
C	-4.131209	-0.577198	-2.449301
H	-3.151144	1.149876	-1.613036
C	-3.136649	-2.724364	-1.941632
H	-1.370003	-2.651993	-0.690719
C	-4.128189	-1.969360	-2.571554
H	-4.898511	0.009295	-2.947756
H	-3.123901	-3.806200	-2.040556
H	-4.893858	-2.463611	-3.163375
C	-0.398703	1.635974	-0.763208
C	-1.079733	2.803133	-0.387065
C	0.593797	1.716222	-1.751843
C	-0.778555	4.022683	-0.995232
H	-1.833694	2.762597	0.393785
C	0.891836	2.934789	-2.361682
H	1.147150	0.820459	-2.024777
C	0.203941	4.089964	-1.985028
H	-1.308961	4.921509	-0.692059
H	1.664703	2.983065	-3.124052
H	0.439203	5.041416	-2.454440
H	3.688990	-4.110591	0.618606
H	2.478998	-4.477807	-0.726344

TS1-a

Free Energy **=** -3964.766561370

Energy = -3965.35917937

C	-4.222306	2.928674	0.961675
O	-5.095519	2.988666	1.807907
O	-4.438877	3.141637	-0.355822
C	-5.805808	3.411540	-0.727743
H	-6.155822	4.295218	-0.183750
H	-6.430191	2.566214	-0.419458
C	-5.834930	3.619375	-2.230579
H	-6.859861	3.825025	-2.558922
H	-5.203334	4.465430	-2.520303
H	-5.476324	2.727185	-2.753811
C	-2.810903	2.595911	1.269116
C	-1.885533	2.366512	0.360100
C	-0.963564	2.102632	-0.547688
H	-2.605687	2.495845	2.333719
Ni	-0.036878	0.402825	-0.255764
P	-0.900843	-1.560099	-0.083464
P	2.024931	0.934494	-0.081634
C	-0.596908	-2.504513	1.480427
C	0.498689	-2.149632	2.280116
C	-1.423744	-3.559346	1.902464
C	0.768855	-2.833859	3.466846
H	1.138635	-1.326893	1.975991
C	-1.153603	-4.244576	3.086943
H	-2.288037	-3.838336	1.306695
C	-0.055640	-3.883389	3.872132
H	1.619099	-2.536621	4.074921
H	-1.803945	-5.057490	3.399854
H	0.149843	-4.413906	4.798335
C	-2.756378	-1.631100	-0.172231
C	-3.476074	-2.283200	-1.182462
C	-3.471242	-0.930465	0.814479
C	-4.872879	-2.227179	-1.209148
H	-2.951326	-2.838018	-1.953426
C	-4.863050	-0.874949	0.789443
H	-2.931632	-0.416255	1.604682
C	-5.569670	-1.523733	-0.227399
H	-5.414332	-2.738904	-2.001109
H	-5.392392	-0.313448	1.554840

H	-6.655379	-1.478985	-0.252686
C	-0.394488	-2.722298	-1.431339
C	-0.410536	-2.229496	-2.748322
C	0.044471	-4.035882	-1.214279
C	-0.011197	-3.030097	-3.817084
H	-0.733873	-1.207224	-2.931594
C	0.457914	-4.833812	-2.284828
H	0.069240	-4.440349	-0.207376
C	0.428386	-4.336303	-3.587578
H	-0.034738	-2.631598	-4.828012
H	0.798063	-5.849135	-2.096730
H	0.748575	-4.958979	-4.418717
C	2.479160	1.225514	1.687274
C	1.735258	2.174214	2.413614
C	3.459129	0.483465	2.362705
C	1.974220	2.380521	3.771332
H	0.967037	2.755817	1.909856
C	3.690167	0.685222	3.726160
H	4.048014	-0.252528	1.824434
C	2.951558	1.633444	4.434028
H	1.392867	3.121729	4.313577
H	4.455903	0.102250	4.231933
H	3.133927	1.789905	5.493846
C	2.525895	2.518449	-0.911538
C	3.211276	3.568219	-0.284009
C	2.166636	2.668696	-2.262295
C	3.525548	4.735227	-0.986096
H	3.502458	3.479638	0.757831
C	2.486629	3.829052	-2.965594
H	1.627038	1.867813	-2.764162
C	3.166623	4.869286	-2.327151
H	4.055204	5.539102	-0.480935
H	2.201109	3.923604	-4.010177
H	3.410839	5.777951	-2.870990
C	3.353810	-0.205809	-0.688802
C	4.633645	0.246583	-1.051096
C	3.077493	-1.576862	-0.782366
C	5.606052	-0.649720	-1.494726
H	4.870215	1.304689	-0.993906
C	4.050547	-2.475162	-1.223909
H	2.091555	-1.942320	-0.516612
C	5.316957	-2.013442	-1.583117
H	6.589955	-0.281530	-1.774389
H	3.809568	-3.532244	-1.297140
H	6.073964	-2.709944	-1.934452
H	-0.422905	2.923272	-1.020048
H	-1.129691	1.140327	-1.195487

TS1-b

Free Energy **=** -2928.487505040

Energy = -2928.82816904

C	-4.456329	0.764696	-0.160978
O	-4.705044	1.930413	-0.406351
O	-5.405473	-0.181793	0.031123
C	-6.766965	0.281257	-0.074024
H	-6.916416	0.726847	-1.063316
H	-6.933775	1.069630	0.667949
C	-7.673837	-0.913829	0.153956
H	-8.722661	-0.604816	0.083047
H	-7.491453	-1.691223	-0.595054
H	-7.507757	-1.347053	1.145598
C	-3.089431	0.221076	-0.039482
C	-2.675090	-1.004026	0.231795
C	-1.927329	-2.140622	0.489715
H	-2.312088	1.011834	-0.207608
Ni	-0.912292	-0.533276	0.109057
H	-1.924225	-2.528601	1.511287
H	-1.923174	-2.934675	-0.260681
P	1.163278	-0.047178	0.018564
C	1.601116	1.632724	-0.609964
C	1.973889	1.848120	-1.944154
C	1.430711	2.743234	0.233379
C	2.182297	3.144119	-2.420483
H	2.105512	1.003922	-2.613973
C	1.641552	4.035877	-0.243819
H	1.136924	2.595430	1.269344
C	2.018813	4.240205	-1.573194
H	2.473881	3.294960	-3.456613
H	1.509359	4.884232	0.422489
H	2.181276	5.247980	-1.945694
C	2.094975	-1.190218	-1.088247
C	3.492932	-1.258360	-1.177863
C	1.318166	-2.037971	-1.889273
C	4.096080	-2.155782	-2.058682
H	4.114412	-0.617943	-0.559179
C	1.920426	-2.930427	-2.776471
H	0.237763	-1.982593	-1.781586
C	3.311900	-2.990073	-2.860880
H	5.180099	-2.205508	-2.119765
H	1.305032	-3.580085	-3.393031
H	3.787161	-3.687197	-3.545963
C	1.992861	-0.121221	1.661699
C	3.247848	0.436706	1.949168
C	1.303929	-0.805499	2.672794
C	3.805320	0.294429	3.220132
H	3.780345	1.003772	1.190775
C	1.861862	-0.949647	3.943018
H	0.319969	-1.202240	2.436296
C	3.116431	-0.402663	4.216363
H	4.776812	0.731743	3.435327
H	1.315383	-1.480859	4.717670
H	3.554001	-0.509751	5.205419

IM2-a

Free Energy **=** -3964.805795500

Energy = -3965.4035175

C	-4.618892	1.897464	-0.004129
O	-5.788932	1.550895	-0.030800
O	-4.247017	3.206605	0.007820
C	-5.327614	4.153552	-0.019210
H	-5.980098	3.983306	0.844614
H	-5.932289	3.986726	-0.917730
C	-4.716973	5.543656	-0.000108
H	-5.507782	6.302237	-0.019771
H	-4.116748	5.693484	0.903431
H	-4.069045	5.696903	-0.869398
C	-3.485288	0.954294	0.022205
C	-2.186539	1.278992	0.065611

C	-1.271680	2.347240	0.095958
H	-3.811275	-0.082857	0.000624
Ni	-0.455433	0.606919	0.085601
H	-1.128020	2.952922	-0.802237
H	-1.172416	2.928869	1.016150
P	1.680233	1.088308	-0.010424
P	-0.743884	-1.567636	0.055383
C	2.554914	0.254327	-1.405063
C	3.680327	-0.566443	-1.262699
C	1.996621	0.413837	-2.687220
C	4.243844	-1.197350	-2.374516
H	4.115729	-0.728107	-0.282839
C	2.566453	-0.207685	-3.797417
H	1.113380	1.035722	-2.816843
C	3.695489	-1.015641	-3.643441
H	5.114271	-1.834613	-2.243283
H	2.127130	-0.063462	-4.781073
H	4.138820	-1.505035	-4.506527
C	2.093757	2.878950	-0.277580
C	1.735048	3.775311	0.743931
C	2.721606	3.387466	-1.421470
C	1.992478	5.138483	0.622692
H	1.251576	3.401622	1.642194
C	2.974741	4.757120	-1.545264
H	3.022789	2.721154	-2.222407
C	2.612073	5.636117	-0.526765
H	1.707420	5.813952	1.425075
H	3.462190	5.131830	-2.441778
H	2.810037	6.700197	-0.624662
C	2.677492	0.772538	1.512645
C	2.044003	0.208040	2.628848
C	4.028405	1.143295	1.621455
C	2.743879	0.002131	3.820421
H	0.992578	-0.061133	2.567537
C	4.730903	0.928883	2.806543
H	4.529036	1.615293	0.780620
C	4.089907	0.356246	3.908573
H	2.233990	-0.430262	4.677142
H	5.776409	1.218170	2.873901
H	4.636630	0.197109	4.834281
C	-1.921108	-2.079476	-1.274636
C	-3.011910	-2.930978	-1.055607
C	-1.720487	-1.557245	-2.563653
C	-3.881233	-3.252998	-2.100618
H	-3.193123	-3.338612	-0.066569
C	-2.580843	-1.890532	-3.608780
H	-0.887395	-0.884078	-2.750321
C	-3.667240	-2.737511	-3.378394
H	-4.729320	-3.905543	-1.910858
H	-2.410354	-1.478610	-4.599959
H	-4.346779	-2.986587	-4.188967
C	-1.474478	-2.242153	1.617023
C	-1.386423	-3.600754	1.966773
C	-2.160940	-1.369838	2.476006
C	-1.966739	-4.070614	3.144882
H	-0.856773	-4.293573	1.320322
C	-2.741497	-1.842072	3.654993
H	-2.254155	-0.322630	2.206894
C	-2.644552	-3.191766	3.993110
H	-1.889366	-5.124480	3.399677
H	-3.271101	-1.151581	4.305846
H	-3.095084	-3.559085	4.911498
C	0.682119	-2.728479	-0.205735
C	1.625997	-2.872630	0.825784
C	0.885590	-3.438830	-1.396332
C	2.731817	-3.707289	0.675169
H	1.491943	-2.338326	1.760906
C	1.998643	-4.269421	-1.550376
H	0.171863	-3.356028	-2.208827
C	2.923129	-4.410306	-0.516616
H	3.442553	-3.809725	1.491335
H	2.134748	-4.813044	-2.481803
H	3.783693	-5.063520	-0.635526

IM2-b

Free Energy = -2928.506141920

Energy = -2928.84825392

C	5.070753	1.356442	-0.382639
O	6.011177	2.117215	-0.539815
O	5.236677	0.039408	-0.083553
C	6.601414	-0.397548	0.035987
H	7.100258	0.186499	0.817413
H	7.128342	-0.196900	-0.903485
C	6.579314	-1.879426	0.365684
H	7.603088	-2.256768	0.468036
H	6.048432	-2.062375	1.305793
H	6.079551	-2.447996	-0.425575
C	3.656875	1.762536	-0.496231
C	2.594472	0.965103	-0.327491
C	2.174770	-0.353526	-0.043989
H	3.545289	2.817136	-0.739115
Ni	0.774542	0.854143	-0.317119
H	2.313241	-1.129614	-0.804280
H	2.260604	-0.748184	0.973231
P	-1.238737	0.075404	-0.049790
C	-2.566292	1.353960	-0.014760
C	-3.190638	1.762204	1.171787
C	-2.875951	2.024716	-1.211033
C	-4.113169	2.810944	1.159680
H	-2.961580	1.260281	2.106580
C	-3.799619	3.068153	-1.220392
H	-2.400266	1.720426	-2.140488
C	-4.421009	3.464745	-0.033313
H	-4.592204	3.114667	2.086721
H	-4.033329	3.572925	-2.153959
H	-5.139065	4.280190	-0.039693
C	-1.416316	-0.819792	1.546950
C	-2.439294	-1.740846	1.816753
C	-0.472798	-0.536759	2.545335
C	-2.519122	-2.356263	3.065790
H	-3.167668	-1.987208	1.049958
C	-0.556868	-1.147922	3.796910
H	0.335297	0.152908	2.317821
C	-1.581430	-2.058518	4.058198
H	-3.312874	-3.071576	3.264188
H	0.181776	-0.919526	4.560292
H	-1.646449	-2.541596	5.029463
C	-1.797275	-1.109438	-1.341004
C	-3.146605	-1.353166	-1.641591

C	-0.806514	-1.812212	-2.043102
C	-3.494133	-2.289160	-2.616391
H	-3.927006	-0.800498	-1.126272
C	-1.155455	-2.750647	-3.014357
H	0.237499	-1.603455	-1.829826
C	-2.500035	-2.991622	-3.301273
H	-4.541966	-2.467325	-2.843300
H	-0.377179	-3.285642	-3.551645
H	-2.773215	-3.718172	-4.061783

TS2-a

Free Energy = -4348.656761810

Energy = -4349.37180281

C	3.784454	2.560349	2.108239
O	3.532871	2.919826	3.240007
O	4.966055	2.789307	1.488488
C	5.950115	3.510187	2.260664
H	6.154245	2.953536	3.181439
H	5.531378	4.479985	2.549695
C	7.188131	3.657716	1.395933
H	7.963400	4.202360	1.946097
H	7.587486	2.677991	1.114918
H	6.960984	4.211339	0.479343
C	2.874983	1.815686	1.193808
C	1.664356	1.481240	1.582217
C	0.500426	1.226623	2.142655
H	3.257115	1.553264	0.210421
Ni	0.100458	0.211940	-0.160158
H	0.360453	0.350064	2.769762
H	-0.297797	1.961682	2.137187
C	3.804739	-0.715291	-2.200821
O	3.881491	0.224162	-2.972621
O	4.759759	-1.692797	-2.142479
C	5.862858	-1.535419	-3.050237
H	6.351711	-0.573085	-2.861127
H	5.483874	-1.507889	-4.078127
C	6.808547	-2.702725	-2.828668
H	7.668257	-2.623659	-3.503702
H	7.178809	-2.714906	-1.798193
H	6.304560	-3.655536	-3.021686
C	2.737034	-0.984081	-1.219392
C	1.672873	-0.175964	-1.094647
C	1.137048	1.006667	-1.620807
H	2.867389	-1.873122	-0.608882
P	-0.460332	-1.808212	0.607448
P	-1.728182	1.473490	-0.532036
H	1.621116	1.962957	-1.419694
H	0.658882	0.982232	-2.601875
C	0.829028	-2.733429	1.579189
C	1.989856	-2.074382	2.005930
C	0.665022	-4.087157	1.919369
C	2.956203	-2.744417	2.762057
H	2.158091	-1.040510	1.726865
C	1.628808	-4.756539	2.670760
H	-0.216995	-4.626962	1.589177
C	2.777577	-4.084959	3.097702
H	3.850079	-2.214170	3.079160
H	1.485046	-5.804728	2.920073
H	3.530183	-4.607864	3.681956
C	-1.918913	-1.931071	1.746977
C	-3.221972	-1.803271	1.232372
C	-1.758850	-2.019887	3.138840
C	-4.327647	-1.790112	2.081495
H	-3.374399	-1.716253	0.161187
C	-2.867387	-1.991729	3.989656
H	-0.766338	-2.126007	3.565442
C	-4.155385	-1.883101	3.464791
H	-5.325137	-1.699054	1.659893
H	-2.719808	-2.065946	5.064093
H	-5.017547	-1.871172	4.126260
C	-3.040498	0.609198	-1.516803
C	-4.411834	0.859927	-1.356373
C	-2.638475	-0.347571	-2.462920
C	-5.354619	0.167990	-2.119265
H	-4.748169	1.592412	-0.629919
C	-3.580649	-1.033902	-3.229944
H	-1.583359	-0.567990	-2.590270
C	-4.942538	-0.779883	-3.057598
H	-6.413136	0.371370	-1.978079
H	-3.246893	-1.776471	-3.949353
H	-5.678122	-1.319954	-3.647910
C	-2.705896	2.279483	0.832399
C	-3.310112	3.540804	0.688810
C	-2.868078	1.602644	2.051792
C	-4.046672	4.104968	1.731430
H	-3.203248	4.090352	-0.240204
C	-3.607964	2.165021	3.093587
H	-2.415676	0.627839	2.192512
C	-4.197713	3.419437	2.937894
H	-4.501746	5.083132	1.598521
H	-3.717500	1.617645	4.025661
H	-4.767871	3.861584	3.750697
C	-1.354073	2.955086	-1.581227
C	-1.873011	3.145456	-2.867220
C	-0.473470	3.919241	-1.061375
C	-1.519461	4.272212	-3.616685
H	-2.555192	2.416632	-3.292433
C	-0.129088	5.045874	-1.803994
H	-0.052142	3.785877	-0.068005
C	-0.650758	5.225009	-3.088572
H	-1.928692	4.400880	-4.615421
H	0.552097	5.780977	-1.383582
H	-0.376863	6.099728	-3.672277
C	-0.885993	-3.050864	-0.712748
C	-1.830650	-4.073534	-0.527099
C	-0.189960	-3.003836	-1.931485
C	-2.081667	-5.009151	-1.532343
H	-2.386761	-4.139524	0.401729
C	-0.436808	-3.943259	-2.933756
H	0.557062	-2.234235	-2.094271
C	-1.386892	-4.947067	-2.740449
H	-2.821776	-5.787965	-1.366649
H	0.118336	-3.887485	-3.866559
H	-1.582064	-5.676162	-3.522589

TS2-b

Free Energy = -3312.381825320

Energy = -3312.83828732

C	3.235862	3.356320	0.050127
O	2.657733	4.325591	0.506019
O	4.576855	3.353782	-0.208236
C	5.267941	4.578872	0.091050
H	5.133182	4.818517	1.151743
H	4.818237	5.395520	-0.484638
C	6.730936	4.377184	-0.261777
H	7.298783	5.289228	-0.045720
H	7.162909	3.555987	0.319717
H	6.847451	4.141766	-1.324786
C	2.643794	2.049103	-0.297526
C	1.338822	1.804010	-0.134595
C	0.127235	2.344993	0.324344
H	3.329056	1.302372	-0.691383
Ni	0.035495	0.518425	-0.301383
H	0.002991	2.541432	1.391368
H	-0.409696	3.062714	-0.299942
P	-2.085600	-0.023081	0.003750
C	-2.742018	-1.511424	-0.875952
C	-3.615887	-1.428426	-1.968909
C	-2.260958	-2.776656	-0.493220
C	-4.006958	-2.581231	-2.654711
H	-3.999796	-0.464068	-2.285916
C	-2.656294	-3.926271	-1.175661
H	-1.578780	-2.861702	0.349000
C	-3.531977	-3.831645	-2.260271
H	-4.688441	-2.498092	-3.497281
H	-2.279202	-4.895926	-0.861448
H	-3.838564	-4.726881	-2.794306
C	-3.249696	1.315983	-0.500751
C	-4.425038	1.625038	0.197683
C	-2.933232	2.055870	-1.651863
C	-5.265221	2.647216	-0.247472
H	-4.684047	1.076147	1.097443
C	-3.779618	3.068467	-2.103374
H	-2.013380	1.844291	-2.191498
C	-4.947458	3.368095	-1.399290
H	-6.168801	2.880482	0.309565
H	-3.519685	3.630299	-2.996390
H	-5.602248	4.164362	-1.742861
C	-2.495962	-0.386053	1.765462
C	-3.601266	-1.164630	2.147134
C	-1.669110	0.147927	2.765827
C	-3.873097	-1.396370	3.495851
H	-4.245047	-1.600684	1.389140
C	-1.942871	-0.083169	4.114552
H	-0.807194	0.741431	2.479821
C	-3.045572	-0.855048	4.482142
H	-4.730996	-2.002076	3.775804
H	-1.290722	0.336904	4.875392
H	-3.257556	-1.038707	5.532058
C	3.850515	-2.892848	-0.537989
O	4.094700	-2.861329	-1.725589
O	4.673344	-3.426738	0.394234
C	5.914390	-3.972647	-0.107601
H	6.459382	-3.181592	-0.632690
H	5.684531	-4.755244	-0.838078
C	6.689834	-4.509129	1.080700
H	7.641557	-4.932634	0.741758
H	6.904079	-3.712272	1.800052
H	6.126486	-5.295030	1.594145
C	2.622136	-2.369752	0.118244
C	1.669337	-1.789759	-0.574158
C	0.717034	-1.212144	-1.267269
H	2.543929	-2.479672	1.197240
H	0.881431	-0.148547	-1.616629
H	-0.044370	-1.799718	-1.774018

IM3-a

Free Energy = -4348.665735570

Energy = -4349.38235357

C	-3.228981	2.679471	-1.967095
O	-2.880628	2.670077	-3.132952
O	-4.303150	3.395460	-1.524300
C	-5.012313	4.137031	-2.533235
H	-5.362090	3.445415	-3.307622
H	-4.322603	4.839610	-3.013956
C	-6.164921	4.851600	-1.850736
H	-6.736452	5.428875	-2.586181
H	-6.841110	4.134569	-1.373779
H	-5.798327	5.539876	-1.081957
C	-2.600148	1.957826	-0.841492
C	-1.492822	1.231580	-1.017535
C	-0.584460	0.739124	-1.940026
H	-3.088260	2.044117	0.124711
Ni	-0.320346	0.099409	-0.024947
H	-0.910647	0.008023	-2.676482
H	0.234353	1.370893	-2.275574
C	-3.802529	-1.634870	1.930751
O	-3.474374	-1.632677	3.103065
O	-5.016351	-2.086510	1.505397
C	-5.901769	-2.557281	2.537950
H	-6.080056	-1.747556	3.253982
H	-5.414571	-3.372452	3.084351
C	-7.185371	-3.012583	1.867258
H	-7.892860	-3.377025	2.620514
H	-7.655505	-2.186757	1.323372
H	-6.989292	-3.822926	1.157436
C	-2.994670	-1.185537	0.777304
C	-1.788672	-0.640860	0.952677
C	-0.869867	-0.222587	1.900655
H	-3.442773	-1.322105	-0.200881
P	0.725185	-1.904421	-0.680402
P	1.328147	1.636309	0.678048
H	-1.070641	0.686833	2.463794
H	-0.272286	-0.961113	2.431674
C	-0.355186	-3.027552	-1.693329
C	-1.619929	-2.616073	-2.130944
C	0.083461	-4.320106	-2.030560
C	-2.425647	-3.467940	-2.891840
H	-1.985905	-1.631429	-1.869911
C	-0.718147	-5.169568	-2.790107
H	1.055408	-4.666964	-1.691712
C	-1.976919	-4.744583	-3.224082
H	-3.404816	-3.128704	-3.218585
H	-0.361941	-6.165599	-3.039936
H	-2.603564	-5.408314	-3.813907
C	2.208986	-1.718182	-1.770533
C	3.438357	-1.296110	-1.233051

C	2.110367	-1.873048	-3.163002
C	4.540766	-1.070928	-2.058660
H	3.539164	-1.134171	-0.165605
C	3.209730	-1.629555	-3.988653
H	1.173337	-2.188853	-3.608639
C	4.430961	-1.235921	-3.440640
H	5.481892	-0.754277	-1.617119
H	3.108583	-1.754560	-5.063552
H	5.288061	-1.055985	-4.084038
C	2.875135	1.010962	1.486125
C	4.110689	1.665991	1.362827
C	2.808253	-0.152017	2.270210
C	5.248510	1.163909	1.997046
H	4.187691	2.569301	0.766770
C	3.944639	-0.649442	2.910679
H	1.866898	-0.679994	2.372982
C	5.169525	0.005667	2.772533
H	6.197455	1.682290	1.885765
H	3.869630	-1.555467	3.505462
H	6.056641	-0.383886	3.264920
C	1.999942	2.800015	-0.599212
C	1.978840	4.196840	-0.469790
C	2.564180	2.243613	-1.760456
C	2.501762	5.012550	-1.475987
H	1.554334	4.654967	0.416648
C	3.093631	3.059330	-2.759907
H	2.597940	1.166016	-1.882488
C	3.060153	4.448214	-2.622705
H	2.472419	6.092651	-1.358145
H	3.525534	2.605468	-3.647731
H	3.464010	5.085344	-3.404987
C	0.652657	2.785515	1.964155
C	1.220356	2.924127	3.238523
C	-0.506476	3.521370	1.659991
C	0.644174	3.775575	4.184705
H	2.113503	2.367812	3.501514
C	-1.073816	4.377173	2.603402
H	-0.968446	3.422012	0.682924
C	-0.501505	4.505514	3.871027
H	1.097132	3.866393	5.168569
H	-1.968635	4.938381	2.347611
H	-0.948150	5.167026	4.608492
C	1.232081	-3.110335	0.639251
C	2.501451	-3.692418	0.765359
C	0.236939	-3.464391	1.569568
C	2.774197	-4.587419	1.803797
H	3.284362	-3.460568	0.051936
C	0.511498	-4.357931	2.603978
H	-0.764126	-3.053109	1.475886
C	1.784446	-4.918928	2.728676
H	3.764246	-5.029855	1.881353
H	-0.272786	-4.613899	3.311070
H	1.999753	-5.613872	3.535989

IM3-b

Free Energy **=** -3312.404884320

Energy = -3312.86544032

C	3.347329	2.915764	0.312959
O	2.860239	3.760143	1.040392
O	4.570284	3.054598	-0.269338
C	5.268211	4.277650	0.032674
H	5.413362	4.348012	1.116258
H	4.646415	5.128053	-0.267759
C	6.588611	4.247518	-0.715513
H	7.154987	5.163231	-0.512157
H	7.194768	3.390561	-0.404128
H	6.424088	4.176364	-1.795671
C	2.742994	1.621832	-0.076282
C	1.537865	1.269620	0.372080
C	0.410287	1.649377	1.076952
H	3.327430	0.985060	-0.731648
Ni	0.242723	-0.066225	0.091766
H	0.393193	1.516310	2.160460
H	-0.197188	2.480317	0.721745
P	-1.999940	0.002727	0.018745
C	-2.828358	-1.126391	-1.189268
C	-3.241703	-0.687205	-2.454819
C	-2.962051	-2.489330	-0.873126
C	-3.776327	-1.587294	-3.379169
H	-3.157513	0.360575	-2.723490
C	-3.499481	-3.385197	-1.796112
H	-2.655143	-2.852849	0.103408
C	-3.907249	-2.937033	-3.054171
H	-4.094491	-1.227423	-4.354028
H	-3.597304	-4.434633	-1.531712
H	-4.324059	-3.635645	-3.774420
C	-2.657248	1.663687	-0.450360
C	-3.785675	2.252817	0.135526
C	-1.968523	2.371862	-1.450539
C	-4.222251	3.512856	-0.278501
H	-4.323715	1.736944	0.923678
C	-2.412148	3.625652	-1.870810
H	-1.071091	1.946854	-1.894478
C	-3.541918	4.199342	-1.284550
H	-5.095503	3.958227	0.190630
H	-1.866980	4.157844	-2.645366
H	-3.883154	5.180453	-1.603168
C	-2.812262	-0.436192	1.612691
C	-4.176226	-0.765999	1.697522
C	-2.040795	-0.447420	2.783789
C	-4.752409	-1.082637	2.927288
H	-4.785678	-0.788959	0.798995
C	-2.617858	-0.767787	4.013812
H	-0.984138	-0.208853	2.727208
C	-3.974675	-1.082189	4.087991
H	-5.808169	-1.334967	2.978205
H	-2.004309	-0.775114	4.910352
H	-4.424725	-1.333344	5.044604
C	3.404051	-2.993428	-0.245532
O	2.881514	-3.875064	-0.900317
O	4.674523	-3.081163	0.236369
C	5.377328	-4.298047	-0.078629
H	5.423832	-4.412770	-1.167064
H	4.811350	-5.149752	0.314310
C	6.759661	-4.200858	0.541172
H	7.331298	-5.110592	0.326023
H	7.309217	-3.344342	0.137319
H	6.693163	-4.084025	1.627805
C	2.798205	-1.702273	0.151485

C	1.554353	-1.391293	-0.211381
C	0.383511	-1.811927	-0.813915
H	3.415048	-1.033161	0.741819
H	0.259643	-1.721593	-1.894553
H	-0.185726	-2.628369	-0.370237

TS3-a

Free Energy = -4348.639533380

Energy = -4349.35633538

Ni	0.078904	0.279287	-0.112880
C	0.679508	0.987914	-1.869636
C	-0.144165	1.192774	1.654237
C	0.950763	1.862951	-0.770721
C	-0.446801	2.012590	0.529185
C	1.915364	2.757973	-0.463197
C	-1.309335	3.018212	0.251394
H	2.026579	3.156500	0.539720
H	-1.452045	3.380750	-0.760731
H	1.560734	0.563383	-2.344886
H	-0.090499	1.257230	-2.588901
H	-0.961766	0.972825	2.333799
H	0.810584	1.350142	2.155530
C	-2.077873	3.702626	1.295706
O	-2.162550	3.393419	2.474546
O	-2.758438	4.760053	0.765790
C	2.846878	3.272681	-1.475530
O	2.900928	2.968744	-2.655268
O	3.709959	4.167429	-0.908559
C	4.673019	4.752337	-1.803285
H	5.284702	3.957713	-2.245248
H	4.144594	5.247939	-2.625018
C	5.510415	5.730037	-0.998338
H	4.883300	6.515826	-0.564886
H	6.031697	5.219643	-0.181552
H	6.259504	6.202107	-1.643839
C	-3.590492	5.489714	1.685084
H	-4.316899	4.803591	2.134733
H	-2.969608	5.883061	2.497501
C	-4.269190	6.600280	0.903359
H	-3.528846	7.274701	0.460809
H	-4.884267	6.189374	0.096022
H	-4.915887	7.185097	1.567045
P	1.724674	-1.166700	0.495441
P	-1.923097	-0.812992	-0.573950
C	-2.900739	-1.286860	0.931515
C	-3.287531	-0.233607	1.781074
C	-3.279763	-2.593124	1.268346
C	-4.016053	-0.485632	2.942185
H	-3.032016	0.792343	1.533631
C	-4.011510	-2.843007	2.433007
H	-3.014574	-3.423623	0.623488
C	-4.377486	-1.793608	3.275240
H	-4.299891	0.344228	3.583503
H	-4.298564	-3.863297	2.674808
H	-4.946138	-1.990546	4.180290
C	-3.253737	0.082787	-1.512669
C	-2.966484	1.225640	-2.269405
C	-4.577002	-0.393894	-1.499778
C	-3.967830	1.875602	-2.996028
H	-1.960969	1.622624	-2.285959
C	-5.576259	0.252371	-2.224619
H	-4.828963	-1.272660	-0.914097
C	-5.274149	1.390951	-2.976159
H	-3.721616	2.763818	-3.571513
H	-6.592660	-0.131956	-2.200068
H	-6.054217	1.897131	-3.538695
C	1.257980	-2.541318	1.648487
C	0.234803	-2.304384	2.581588
C	1.880029	-3.800028	1.638625
C	-0.144748	-3.293710	3.490871
H	-0.275093	-1.346546	2.585303
C	1.492883	-4.790430	2.542647
H	2.663748	-4.014485	0.919973
C	0.483059	-4.539601	3.473679
H	-0.942474	-3.089793	4.199497
H	1.983530	-5.760162	2.518182
H	0.183712	-5.312953	4.176235
C	2.675009	-2.011546	-0.849650
C	4.000119	-2.450407	-0.677606
C	2.048578	-2.239631	-2.083812
C	4.673374	-3.104676	-1.709092
H	4.512403	-2.269780	0.262428
C	2.722760	-2.896980	-3.115013
H	1.032657	-1.895258	-2.242369
C	4.035171	-3.330621	-2.930808
H	5.698241	-3.434064	-1.558832
H	2.219351	-3.062228	-4.063546
H	4.562278	-3.835832	-3.735923
C	3.067456	-0.302522	1.428163
C	3.154109	-0.344990	2.827522
C	3.967773	0.513929	0.722295
C	4.121418	0.402546	3.502349
H	2.470843	-0.966830	3.396775
C	4.933144	1.259081	1.398893
H	3.922266	0.560534	-0.360975
C	5.012923	1.206493	2.791582
H	4.176200	0.352887	4.586745
H	5.614352	1.889816	0.834555
H	5.763207	1.789687	3.318761
C	-1.756770	-2.377729	-1.548193
C	-1.060538	-3.465431	-0.992429
C	-2.218796	-2.486045	-2.869131
C	-0.860824	-4.636040	-1.723547
H	-0.668037	-3.398877	0.016788
C	-2.002296	-3.653008	-3.605568
H	-2.751998	-1.660686	-3.328241
C	-1.330638	-4.734129	-3.034584
H	-0.326083	-5.465612	-1.268942
H	-2.366923	-3.715277	-4.627647
H	-1.169736	-5.643491	-3.607453

TS3-b

Free Energy = -3312.378884560

Energy = -3312.83905256

Ni	0.255290	-0.047063	0.017751
C	1.020903	0.881010	1.566816
C	0.996875	-0.987242	-1.527554
C	1.888191	0.798395	0.434415

C	1.878454	-0.913368	-0.405702
C	2.757247	1.604555	-0.213622
C	2.749826	-1.725109	0.230023
H	3.078355	1.397854	-1.229476
H	3.087612	-1.522540	1.241282
H	0.757082	1.885960	1.888501
H	1.194273	0.198208	2.401047
H	0.698795	-1.989505	-1.826318
H	1.183515	-0.317655	-2.370275
P	-1.911181	-0.016335	0.015480
C	3.323741	-2.909990	-0.430191
O	3.089287	-3.308056	-1.556907
O	4.180393	-3.545428	0.417170
C	3.351459	2.785008	0.435651
O	3.114475	3.204528	1.554512
O	4.228657	3.390895	-0.412002
C	4.873755	4.573083	0.099156
H	4.109445	5.315868	0.353209
H	5.401800	4.320028	1.024795
C	5.820331	5.077371	-0.974966
H	6.575446	4.322005	-1.215374
H	5.275779	5.322362	-1.892723
H	6.333803	5.980410	-0.626619
C	4.803001	-4.735233	-0.104159
H	4.024171	-5.455656	-0.377405
H	5.347448	-4.481475	-1.020108
C	5.725219	-5.277456	0.972695
H	6.495186	-4.543869	1.232754
H	5.164531	-5.523053	1.880530
H	6.221174	-6.187243	0.616597
C	-2.762827	-1.311974	-0.982174
C	-2.410549	-1.437313	-2.336843
C	-3.708544	-2.193830	-0.442514
C	-3.002062	-2.414085	-3.134492
H	-1.665420	-0.771640	-2.762767
C	-4.291987	-3.179985	-1.242602
H	-3.992632	-2.116389	0.601789
C	-3.943305	-3.290926	-2.587771
H	-2.721570	-2.497518	-4.180961
H	-5.020603	-3.860096	-0.809412
H	-4.397543	-4.058808	-3.208131
C	-2.704981	-0.130596	1.672933
C	-3.930375	0.480663	1.975791
C	-2.052938	-0.878823	2.664347
C	-4.492330	0.340617	3.245607
H	-4.442567	1.074854	1.224920
C	-2.620337	-1.025808	3.929965
H	-1.090027	-1.331822	2.444733
C	-3.840985	-0.414546	4.222699
H	-5.438496	0.825001	3.471815
H	-2.104262	-1.607857	4.688553
H	-4.279719	-0.520068	5.211273
C	-2.519887	1.567475	-0.699894
C	-3.710835	1.664904	-1.434850
C	-1.764001	2.727817	-0.468567
C	-4.137179	2.900568	-1.924887
H	-4.300927	0.775421	-1.633019
C	-2.193396	3.961002	-0.957752
H	-0.835350	2.657056	0.089928
C	-3.381153	4.049533	-1.686450
H	-5.059948	2.963473	-2.495521
H	-1.596572	4.850047	-0.773871
H	-3.713674	5.009644	-2.071812

IM4-a

Free Energy = -4348.699566170

Energy = -4349.42090817

Ni	0.271395	-0.002327	-0.110441
C	1.760083	1.169292	0.523425
C	1.734221	-1.180506	-0.713994
C	3.007872	0.731339	-0.125557
C	2.989696	-0.750739	-0.080406
C	3.971894	1.426457	-0.780011
C	3.922386	-1.468813	0.593635
H	4.813819	0.892119	-1.209821
H	4.785798	-0.962000	1.014105
H	1.621916	2.249713	0.502846
H	1.801932	0.838948	1.571476
H	1.573663	-2.253293	-0.643202
H	1.771452	-0.898365	-1.779199
P	-1.117522	1.567870	0.751852
P	-1.168217	-1.557595	-0.790050
C	3.845458	-2.909182	0.849923
O	2.897123	-3.660378	0.666202
O	5.021936	-3.357049	1.379246
C	3.967557	2.875678	-0.987282
O	3.072784	3.670026	-0.735707
O	5.147170	3.276112	-1.550099
C	5.266361	4.683339	-1.815251
H	4.451507	4.996762	-2.477784
H	5.151743	5.238582	-0.877586
C	6.627899	4.915664	-2.446356
H	7.429591	4.597176	-1.772082
H	6.725052	4.354949	-3.381838
H	6.763894	5.980688	-2.665914
C	5.073337	-4.757713	1.697847
H	4.283423	-4.992860	2.420302
H	4.868803	-5.341229	0.793361
C	6.454946	-5.048001	2.256990
H	7.230821	-4.806444	1.523184
H	6.642949	-4.457847	3.159969
H	6.541044	-6.109825	2.513931
C	-1.811961	-2.447621	0.685601
C	-0.867519	-3.146059	1.465975
C	-3.137846	-2.374876	1.132578
C	-1.259659	-3.784357	2.642007
H	0.174229	-3.198728	1.158182
C	-3.522255	-3.014194	2.313960
H	-3.874585	-1.808202	0.574406
C	-2.589312	-3.725132	3.067318
H	-0.521008	-4.326641	3.225997
H	-4.555283	-2.946377	2.644358
H	-2.892283	-4.223331	3.984522
C	-2.586592	-1.052206	-1.862390
C	-2.444853	0.125794	-2.610067
C	-3.706123	-1.866565	-2.095689
C	-3.408921	0.495865	-3.550939
H	-1.579237	0.763860	-2.450141
C	-4.678675	-1.488046	-3.020301

H	-3.814676	-2.806686	-1.563509
C	-4.533066	-0.305373	-3.750236
H	-3.280150	1.411173	-4.122487
H	-5.544452	-2.124912	-3.181880
H	-5.287041	-0.017734	-4.478179
C	-2.918437	1.254195	1.120785
C	-3.882035	1.406937	0.109500
C	-3.355887	0.842887	2.389161
C	-5.230871	1.149241	0.353712
H	-3.585217	1.743368	-0.876113
C	-4.706769	0.590652	2.636313
H	-2.647810	0.728919	3.201371
C	-5.650373	0.738758	1.620341
H	-5.952280	1.276343	-0.449025
H	-5.017951	0.281905	3.630936
H	-6.702211	0.545688	1.814633
C	-0.508972	2.082978	2.423668
C	-0.337827	3.418894	2.805121
C	-0.187801	1.070165	3.344457
C	0.129722	3.736683	4.082705
H	-0.555129	4.217876	2.104527
C	0.268461	1.389691	4.622797
H	-0.281864	0.024907	3.058050
C	0.428690	2.726074	4.995487
H	0.264733	4.779027	4.359095
H	0.511006	0.593878	5.321926
H	0.794176	2.975947	5.987904
C	-1.203046	3.123758	-0.243329
C	-2.163649	4.121465	0.003460
C	-0.269944	3.328763	-1.270820
C	-2.189713	5.287210	-0.760834
H	-2.900570	3.983893	0.788694
C	-0.294497	4.499471	-2.031418
H	0.498105	2.588034	-1.462095
C	-1.254634	5.478404	-1.781411
H	-2.939597	6.047182	-0.557034
H	0.450015	4.644285	-2.808617
H	-1.273767	6.389563	-2.373667
C	-0.543838	-2.909956	-1.899570
C	-0.583673	-4.273107	-1.585593
C	-0.049758	-2.523145	-3.156423
C	-0.128710	-5.225662	-2.501641
H	-0.965084	-4.604147	-0.626302
C	0.403471	-3.472650	-4.068290
H	-0.022476	-1.470945	-3.427158
C	0.367095	-4.830591	-3.742190
H	-0.162989	-6.279290	-2.237312
H	0.786252	-3.152579	-5.033791
H	0.723057	-5.572974	-4.451493

IM4-b

Free Energy **=** -3312.413626440

Energy = -3312.87738944

Ni	-0.207269	-0.220562	-0.449846
C	1.497610	-0.771881	-1.169906
C	0.759614	1.012856	0.647494
C	2.575545	-0.242138	-0.301458
C	2.163908	1.101473	0.173355
C	3.705766	-0.841657	0.148100
C	2.959805	2.189581	0.033783
H	4.351147	-0.310030	0.840944
H	3.952377	2.072779	-0.390754
H	1.586126	-1.839530	-1.378303
H	1.517036	-0.217896	-2.124330
H	0.285580	1.985434	0.780880
H	0.758340	0.485058	1.617668
P	-2.305868	-0.065897	0.158768
C	2.585803	3.562156	0.398246
O	1.520212	3.960225	0.841773
O	3.633689	4.406949	0.168520
C	4.147836	-2.193744	-0.213706
O	3.585134	-3.005038	-0.931311
O	5.346361	-2.465602	0.383923
C	5.902563	-3.761745	0.105915
H	5.198004	-4.534223	0.434255
H	6.026771	-3.876204	-0.976689
C	7.228073	-3.856657	0.840479
H	7.919218	-3.078643	0.500055
H	7.085564	-3.738979	1.919757
H	7.690247	-4.833305	0.657590
C	3.401543	5.789745	0.487851
H	2.551278	6.156407	-0.098060
H	3.126521	5.873887	1.545103
C	4.676330	6.551808	0.172409
H	5.514620	6.172733	0.766051
H	4.936277	6.456262	-0.886918
H	4.544178	7.615302	0.401208
C	-3.582859	0.916347	-0.702693
C	-3.544160	2.311573	-0.549911
C	-4.579575	0.340923	-1.507595
C	-4.494236	3.115819	-1.179743
H	-2.762073	2.766478	0.052463
C	-5.522839	1.149302	-2.142496
H	-4.607971	-0.736198	-1.646743
C	-5.483697	2.535717	-1.975769
H	-4.454621	4.194428	-1.056458
H	-6.287755	0.696901	-2.767938
H	-6.219046	3.162995	-2.472281
C	-1.917037	-1.506076	-0.890475
C	-1.899722	-2.850748	-0.446751
C	-1.365392	-1.190909	-2.159648
C	-1.370943	-3.844565	-1.253285
H	-2.305547	-3.097866	0.529531
C	-0.864374	-2.225136	-2.974868
H	-1.520372	-0.211067	-2.605208
C	-0.846427	-3.533244	-2.521543
H	-1.367229	-4.873903	-0.905347
H	-0.481454	-1.985419	-3.962700
H	-0.438966	-4.322484	-3.146435
C	-3.034268	-0.685999	1.716700
C	-4.416828	-0.727758	1.951735
C	-2.153787	-1.116130	2.723389
C	-4.908322	-1.205571	3.166607
H	-5.108543	-0.382306	1.189585
C	-2.650087	-1.602689	3.932614
H	-1.080777	-1.066611	2.558677
C	-4.027535	-1.646779	4.156261
H	-5.980741	-1.232515	3.339814
H	-1.960112	-1.935477	4.702963

H	-4.413513	-2.017322	5.102001

TS4-a

Free Energy = -4348.658789120

Energy = -4349.37273912

Ni	0.301787	0.147046	-0.264855
C	-0.969939	0.241428	-1.801723
C	-0.708443	1.779977	-0.712410
C	-2.414514	0.557505	-1.527723
C	-2.210323	1.833863	-0.842814
C	-3.555594	-0.125345	-1.761510
C	-3.087832	2.789004	-0.471977
H	-4.508818	0.274303	-1.428458
H	-4.151768	2.669593	-0.653779
H	-0.637082	0.673749	-2.751598
H	-0.689073	-0.828023	-1.802500
H	-0.359185	1.844131	0.347500
H	-0.189614	2.538679	-1.302706
P	-0.313044	-1.215596	1.339703
P	2.359343	0.520309	-0.836312
C	-2.658286	4.019688	0.205237
O	-1.511855	4.316440	0.503080
O	-3.722559	4.818071	0.479644
C	-3.591606	-1.428834	-2.434356
O	-2.629367	-2.096023	-2.786862
O	-4.872771	-1.833240	-2.628357
C	-5.038594	-3.107990	-3.281147
H	-4.536314	-3.078102	-4.253873
H	-4.545112	-3.880888	-2.681944
C	-6.528883	-3.360160	-3.417581
H	-7.013019	-3.381850	-2.435887
H	-7.004188	-2.577636	-4.017833
H	-6.700871	-4.324226	-3.908805
C	-3.419085	6.058235	1.150051
H	-2.906913	5.837119	2.092632
H	-2.726180	6.637238	0.530117
C	-4.729769	6.790086	1.372955
H	-5.227664	6.999336	0.420647
H	-5.409162	6.195803	1.992581
H	-4.543286	7.742434	1.881401
C	3.339972	1.556062	0.351546
C	2.731456	2.702716	0.894794
C	4.630011	1.217849	0.787521
C	3.398814	3.493472	1.829520
H	1.726623	2.982942	0.589389
C	5.291506	2.002438	1.736024
H	5.123595	0.337017	0.390563
C	4.681392	3.143237	2.257516
H	2.909779	4.377384	2.230250
H	6.289717	1.720432	2.061903
H	5.198189	3.753036	2.993899
C	3.495139	-0.898679	-1.196685
C	3.256857	-2.128427	-0.567419
C	4.594422	-0.791984	-2.065982
C	4.090467	-3.224564	-0.798150
H	2.407892	-2.232332	0.100014
C	5.426788	-1.886890	-2.298815
H	4.795951	0.148914	-2.569305
C	5.176301	-3.106902	-1.665647
H	3.878404	-4.169860	-0.305965
H	6.270665	-1.787357	-2.976928
H	5.822425	-3.960863	-1.852494
C	0.538154	-1.058593	2.982928
C	1.863412	-0.601738	3.016432
C	-0.081275	-1.400901	4.196571
C	2.552170	-0.484237	4.224966
H	2.359053	-0.330529	2.090467
C	0.604941	-1.281535	5.405528
H	-1.106557	-1.757387	4.199258
C	1.923321	-0.820998	5.423835
H	3.575460	-0.118453	4.223499
H	0.107173	-1.547730	6.334688
H	2.454488	-0.723294	6.367218
C	-2.092532	-1.127270	1.877061
C	-2.985462	-2.206916	1.843979
C	-2.568830	0.119926	2.317704
C	-4.319085	-2.041614	2.229231
H	-2.643613	-3.183586	1.517975
C	-3.895028	0.282387	2.712539
H	-1.894547	0.972687	2.353562
C	-4.778378	-0.799612	2.665554
H	-4.996599	-2.891196	2.192267
H	-4.240667	1.255351	3.052428
H	-5.815108	-0.673378	2.966538
C	-0.097166	-3.013269	0.936634
C	0.645957	-3.893998	1.737285
C	-0.650846	-3.501547	-0.261142
C	0.836128	-5.223029	1.348724
H	1.081394	-3.545515	2.667969
C	-0.470709	-4.831630	-0.639495
H	-1.231672	-2.849600	-0.908011
C	0.278202	-5.697152	0.161368
H	1.416935	-5.888339	1.983002
H	-0.911424	-5.184851	-1.567985
H	0.425896	-6.731401	-0.138585
C	2.481153	1.476267	-2.424396
C	2.854431	2.825301	-2.503786
C	2.057932	0.831144	-3.601864
C	2.810598	3.507635	-3.723260
H	3.189758	3.350339	-1.615193
C	2.022606	1.509805	-4.818533
H	1.765761	-0.215820	-3.566491
C	2.397277	2.854750	-4.883592
H	3.107512	4.552773	-3.762147
H	1.700737	0.988469	-5.716512
H	2.365572	3.386777	-5.830685

TS4-b

Free Energy = -3312.376223500

Energy = -3312.83463950

Ni	-0.004501	-0.388435	0.653808
C	-1.737119	-1.112732	0.944377
C	-1.342600	0.664193	1.499644
C	-2.990753	-0.431075	0.498098
C	-2.542801	0.954926	0.638794
C	-4.221381	-0.922753	0.226463
C	-3.034904	2.101100	0.126350
H	-5.041044	-0.251032	-0.009228

H	-3.920633	2.081619	-0.501956
H	-1.115418	-1.559443	0.082709
H	-1.837434	-1.898087	1.694072
H	-1.560878	0.670184	2.570166
H	-0.417212	1.287114	1.352472
C	-2.399534	3.409827	0.335381
O	-1.331286	3.618201	0.888849
O	-3.158422	4.401011	-0.198143
C	-4.512921	-2.359477	0.237368
O	-3.722461	-3.254781	0.491597
O	-5.812698	-2.591423	-0.088608
C	-6.211731	-3.975957	-0.121141
H	-5.587022	-4.510126	-0.845228
H	-6.027003	-4.423465	0.861393
C	-7.681305	-4.018992	-0.497971
H	-8.288821	-3.478617	0.235250
H	-7.846380	-3.566331	-1.481138
H	-8.027195	-5.057937	-0.534067
C	-2.631180	5.736914	-0.064448
H	-2.475931	5.953147	0.997794
H	-1.651856	5.782871	-0.553192
C	-3.628875	6.687629	-0.699732
H	-3.772182	6.453858	-1.759657
H	-4.600745	6.625484	-0.199647
H	-3.265004	7.717880	-0.619582
P	2.034808	-0.448243	0.026014
C	3.269569	-0.223976	1.380766
C	4.074208	0.916759	1.498755
C	3.336986	-1.207719	2.382896
C	4.931085	1.068196	2.592057
H	4.033341	1.691034	0.739354
C	4.197881	-1.058266	3.467986
H	2.713174	-2.095515	2.310145
C	4.997555	0.082992	3.576567
H	5.547787	1.959793	2.670428
H	4.241343	-1.830153	4.231918
H	5.664779	0.202868	4.425910
C	2.618707	-1.983919	-0.821941
C	3.935507	-2.460778	-0.736241
C	1.700539	-2.679470	-1.622605
C	4.321508	-3.606456	-1.435010
H	4.659242	-1.945348	-0.112156
C	2.087660	-3.819086	-2.326589
H	0.672018	-2.331247	-1.676421
C	3.400249	-4.286192	-2.233168
H	5.343438	-3.967708	-1.353145
H	1.361780	-4.347204	-2.939040
H	3.701469	-5.179516	-2.773872
C	2.427208	0.881512	-1.193798
C	1.550421	1.974153	-1.257335
C	3.543658	0.855464	-2.043144
C	1.788513	3.027335	-2.140836
H	0.676890	1.985532	-0.612253
C	3.778057	1.905718	-2.930859
H	4.225292	0.010189	-2.021276
C	2.903198	2.994322	-2.979500
H	1.099898	3.867172	-2.172945
H	4.643752	1.873186	-3.587363
H	3.088985	3.810414	-3.672931

IM5-a'

Free Energy = -4732.574602540

Energy = -4733.40396754

Ni	1.239277	0.037818	0.678146
C	2.032969	1.250488	-0.686649
C	1.147270	1.683084	1.763587
C	2.466418	2.503710	-0.047242
C	1.434483	2.881905	0.946713
C	3.630569	3.193727	-0.162954
C	0.860011	4.108458	0.950929
H	3.773577	4.093353	0.427466
H	1.210877	4.859478	0.249566
H	2.735053	0.856935	-1.417527
H	1.066282	1.426647	-1.191430
H	0.257326	1.780398	2.385269
H	2.019886	1.501489	2.410689
P	1.764945	-1.744020	-0.711334
P	-3.424120	0.199245	-0.910423
C	-0.221240	4.542082	1.844134
O	-0.886950	3.854526	2.605520
O	-0.415008	5.883585	1.714987
C	4.754281	2.812732	-1.021933
O	4.902717	1.767135	-1.639987
O	5.689305	3.803576	-1.046371
C	6.856394	3.545710	-1.847984
H	7.352545	2.641163	-1.478606
H	6.546721	3.347462	-2.879824
C	7.756214	4.764479	-1.750210
H	7.244854	5.657885	-2.123023
H	8.054093	4.948015	-0.712747
H	8.661719	4.610228	-2.347589
C	-1.444677	6.464341	2.535617
H	-2.417387	6.076155	2.212588
H	-1.293931	6.155005	3.574997
C	-1.362541	7.971527	2.372010
H	-0.386687	8.345889	2.697792
H	-1.508946	8.259610	1.325957
H	-2.137783	8.456539	2.975636
C	-4.247998	0.149631	-2.571570
C	-3.776487	1.052462	-3.541944
C	-5.261205	-0.749966	-2.932742
C	-4.314300	1.067222	-4.828336
H	-2.985560	1.753962	-3.284423
C	-5.792009	-0.742708	-4.225662
H	-5.638986	-1.460293	-2.203721
C	-5.323694	0.165268	-5.175292
H	-3.943051	1.779580	-5.560774
H	-6.576961	-1.447913	-4.487428
H	-5.739024	0.169772	-6.179580
C	-4.183289	-1.243224	-0.027299
C	-3.530262	-2.481671	-0.149785
C	-5.329204	-1.169201	0.779548
C	-4.017389	-3.617212	0.497822
H	-2.629223	-2.559925	-0.753721
C	-5.812316	-2.303816	1.434754
H	-5.843970	-0.221522	0.903449
C	-5.160862	-3.530233	1.294105
H	-3.491964	-4.562214	0.390246
H	-6.699763	-2.226844	2.057972

H	-5.537621	-4.410743	1.808127
C	0.845436	-3.331680	-0.462193
C	0.966674	-3.992407	0.773742
C	0.031830	-3.905596	-1.450909
C	0.295572	-5.190971	1.010809
H	1.593926	-3.571026	1.551971
C	-0.640235	-5.107268	-1.210623
H	-0.071326	-3.425277	-2.417490
C	-0.510501	-5.753855	0.018669
H	0.406150	-5.685698	1.971839
H	-1.257548	-5.539949	-1.993517
H	-1.027456	-6.692296	0.200973
C	1.485942	-1.372040	-2.491788
C	2.460467	-1.588049	-3.474566
C	0.239723	-0.841510	-2.868347
C	2.191036	-1.285857	-4.811159
H	3.432543	-1.983670	-3.199079
C	-0.030166	-0.553745	-4.205987
H	-0.526162	-0.648320	-2.119711
C	0.946915	-0.774176	-5.179837
H	2.958268	-1.450700	-5.562819
H	-1.002074	-0.153595	-4.481709
H	0.739972	-0.541893	-6.221096
C	3.529931	-2.264420	-0.580641
C	3.922141	-3.604266	-0.741187
C	4.516528	-1.293238	-0.341663
C	5.266490	-3.964391	-0.649533
H	3.178601	-4.370404	-0.933066
C	5.860993	-1.658371	-0.259971
H	4.252953	-0.246756	-0.248710
C	6.239072	-2.992906	-0.406069
H	5.552203	-5.005942	-0.770632
H	6.608495	-0.889844	-0.086343
H	7.285990	-3.275765	-0.334896
C	-4.238353	1.653174	-0.107326
C	-5.512164	2.133448	-0.454087
C	-3.528483	2.301228	0.915452
C	-6.066408	3.221929	0.220669
H	-6.069825	1.657073	-1.255380
C	-4.087916	3.381785	1.599697
H	-2.526262	1.974312	1.179520
C	-5.358821	3.842832	1.253276
H	-7.052678	3.584008	-0.059198
H	-3.512454	3.856759	2.388000
H	-5.795455	4.688117	1.779421
C	1.649252	-2.094087	4.448058
O	2.507198	-2.398580	5.254692
O	0.341979	-2.410627	4.588296
C	-0.001573	-3.124591	5.794669
H	0.324486	-2.537641	6.659447
H	0.548081	-4.071947	5.815604
C	-1.503851	-3.337493	5.784302
H	-1.808976	-3.881815	6.684895
H	-2.033246	-2.379681	5.763396
H	-1.811340	-3.917757	4.908289
C	1.936551	-1.336767	3.205083
C	1.018190	-0.990617	2.311851
C	-0.220532	-0.875505	1.758089
H	2.984844	-1.081142	3.077795
H	-0.922885	-0.131206	2.125092
H	-0.656219	-1.708615	1.210632

IM5-b

Free Energy **=** -3312.425594440

Energy = -3312.89495744

Ni	0.306205	-1.128248	-0.148879
P	-0.104951	0.944997	0.142194
C	-1.648348	1.651718	-0.580618
C	-1.820724	1.551892	-1.970066
C	-2.634581	2.295831	0.179409
C	-2.946660	2.093272	-2.587724
H	-1.070932	1.043939	-2.571913
C	-3.768126	2.829179	-0.439126
H	-2.523038	2.377509	1.256049
C	-3.924940	2.733417	-1.822260
H	-3.062977	2.011382	-3.665077
H	-4.526050	3.323832	0.162757
H	-4.804850	3.153566	-2.302216
C	-0.372654	0.977525	1.965181
C	0.380520	1.780325	2.832779
C	-1.333206	0.100295	2.504735
C	0.175237	1.714232	4.212587
H	1.130454	2.455828	2.434650
C	-1.539038	0.045837	3.882794
H	-1.922765	-0.541882	1.855394
C	-0.784933	0.850703	4.740127
H	0.768673	2.340055	4.873948
H	-2.285824	-0.633482	4.284586
H	-0.942738	0.801229	5.814236
C	1.128267	2.273181	-0.195779
C	0.801047	3.637432	-0.117629
C	2.434261	1.904558	-0.544563
C	1.766511	4.610697	-0.370282
H	-0.211451	3.939784	0.134259
C	3.399152	2.881971	-0.798526
H	2.690501	0.853438	-0.631639
C	3.068726	4.234011	-0.710285
H	1.501813	5.662941	-0.306973
H	4.407933	2.583242	-1.070689
H	3.819409	4.993794	-0.911629
C	1.255076	-3.808501	0.983204
C	1.142621	-2.922824	-0.254416
C	-0.294221	-3.013895	-0.256146
C	-0.305141	-3.909786	0.978211
H	1.786604	-4.747557	0.798544
H	1.698692	-3.329871	1.858934
H	-0.704701	-4.911054	0.783561
H	-0.813592	-3.497870	1.852318
C	-1.244715	-2.159644	-0.878786
C	2.011717	-1.976237	-0.860032
C	3.408131	-1.903791	-0.403678
O	3.883964	-2.424624	0.590116
O	4.157611	-1.135216	-1.251754
C	-2.641140	-2.160500	-0.407032
O	-3.032849	-2.487879	0.703657
O	-3.481279	-1.701035	-1.368929
C	5.547266	-0.996830	-0.897229
H	5.622725	-0.461606	0.056148
H	5.978163	-1.991526	-0.746135

C	6.236022	-0.248207	-2.024123
H	7.297920	-0.113720	-1.790148
H	6.157364	-0.802043	-2.965258
H	5.788648	0.740458	-2.173464
C	-4.867339	-1.586395	-0.988469
H	-4.948480	-0.879742	-0.155457
H	-5.220681	-2.558930	-0.630715
C	-5.637454	-1.113121	-2.207361
H	-5.539901	-1.826625	-3.032230
H	-6.700726	-1.013955	-1.961614
H	-5.267155	-0.140059	-2.544966
H	-1.144001	-1.928555	-1.939707
H	1.873914	-1.694573	-1.903975

TS5-b

Free Energy **=** -3312.417885710

Energy = -3312.88347271

Ni	0.059882	0.539941	-0.994523
P	1.382678	-0.924949	-0.103114
C	0.335580	-2.290033	0.550660
C	-1.017527	-1.983348	0.752942
C	0.791526	-3.585415	0.839686
C	-1.900383	-2.935963	1.259355
H	-1.363833	-0.987164	0.495676
C	-0.091997	-4.540634	1.344695
H	1.828702	-3.853427	0.658260
C	-1.435274	-4.217380	1.558832
H	-2.944911	-2.672783	1.403316
H	0.267559	-5.541997	1.566756
H	-2.117600	-4.968117	1.948556
C	2.629818	-1.786935	-1.154759
C	4.006389	-1.550553	-1.043388
C	2.167544	-2.633196	-2.177233
C	4.901241	-2.151925	-1.931434
H	4.383965	-0.897115	-0.263107
C	3.062561	-3.234992	-3.059572
H	1.102689	-2.830781	-2.278366
C	4.433845	-2.995167	-2.939200
H	5.966393	-1.960573	-1.831234
H	2.689717	-3.890642	-3.842000
H	5.131817	-3.462059	-3.628762
C	2.344654	-0.298765	1.332856
C	2.695103	-1.094174	2.433644
C	2.767077	1.037655	1.292947
C	3.461169	-0.560696	3.470067
H	2.360827	-2.125311	2.489028
C	3.541278	1.566641	2.326020
H	2.461931	1.662309	0.459995
C	3.889993	0.767634	3.415729
H	3.722141	-1.183126	4.321845
H	3.861723	2.603891	2.282811
H	4.486190	1.179931	4.225376
C	-1.703406	2.331984	-2.646637
C	-1.377583	1.783205	-1.244365
C	-2.734870	1.240410	-1.105244
C	-3.085033	1.609872	-2.538056
H	-1.768424	3.424175	-2.684034
H	-1.055563	2.010655	-3.469256
H	-3.973137	2.240935	-2.632692
H	-3.220608	0.749542	-3.202360
C	-3.436722	0.672406	-0.096800
C	-0.443716	2.182563	-0.226477
C	0.449986	3.323146	-0.516551
O	0.825418	3.685490	-1.619168
O	0.836115	3.954786	0.626080
C	-4.803527	0.188789	-0.282996
O	-5.477310	0.272884	-1.297354
O	-5.265055	-0.411910	0.856375
C	1.702380	5.093561	0.448674
H	2.627509	4.767778	-0.040252
H	1.217348	5.810430	-0.221711
C	1.962816	5.687000	1.821272
H	2.626310	6.554586	1.734684
H	1.028099	6.012332	2.289113
H	2.436746	4.953514	2.482279
C	-6.612426	-0.914109	0.789318
H	-6.679775	-1.658501	-0.011812
H	-7.288257	-0.093248	0.526130
C	-6.948671	-1.508945	2.145011
H	-6.873885	-0.752351	2.932886
H	-7.971844	-1.900955	2.138841
H	-6.267887	-2.330202	2.393427
H	-3.000904	0.555453	0.891581
H	-0.754198	2.112903	0.816930

TS6-b

Free Energy **=** -3696.290014970

Energy = -3696.86515097

Ni	0.242855	0.068059	-0.461456
C	2.100484	0.359490	-0.553809
C	0.030220	1.968252	-0.249385
C	2.353282	1.630585	0.165575
C	1.357692	2.627124	-0.303957
C	3.218023	1.891035	1.177228
C	1.723032	3.829792	-0.805608
H	3.254535	2.891697	1.596898
H	2.772873	4.107210	-0.825852
H	2.733233	-0.463804	-0.225212
H	2.245657	0.527543	-1.633712
H	-0.716339	2.456243	-0.880457
H	-0.328547	1.998399	0.798261
P	0.193060	-2.143830	-0.623101
C	0.793137	4.819506	-1.366839
O	-0.415289	4.718993	-1.503822
O	1.476264	5.937546	-1.747838
C	4.114491	0.912050	1.800541
O	4.129217	-0.301746	1.642161
O	4.976011	1.536783	2.648284
C	5.906748	0.685986	3.343184
H	5.347732	-0.038115	3.946541
H	6.489593	0.118203	2.610059
C	6.786468	1.577442	4.200895
H	7.335724	2.294489	3.582264
H	6.186617	2.138087	4.925109
H	7.512527	0.968702	4.751184
C	0.679296	6.993721	-2.313002
H	0.142974	6.610313	-3.188051
H	-0.074528	7.305367	-1.581512

C	1.618152	8.129923	-2.677082
H	2.147405	8.497854	-1.792037
H	2.362773	7.801830	-3.409755
H	1.050375	8.961048	-3.110167
C	-1.551493	-2.643631	-0.956980
C	-2.485208	-2.590249	0.092525
C	-2.000901	-2.956646	-2.248037
C	-3.833010	-2.859365	-0.142394
H	-2.156771	-2.348027	1.099644
C	-3.352215	-3.220820	-2.481320
H	-1.295816	-3.001122	-3.072084
C	-4.270707	-3.174816	-1.431272
H	-4.540804	-2.818041	0.680761
H	-3.684918	-3.468014	-3.485945
H	-5.321125	-3.383423	-1.614850
C	1.145184	-2.833243	-2.038139
C	1.643764	-4.143537	-2.068621
C	1.366197	-1.993883	-3.141391
C	2.339007	-4.605838	-3.186289
H	1.498712	-4.800475	-1.216602
C	2.054082	-2.460597	-4.261893
H	1.010949	-0.967350	-3.106602
C	2.541714	-3.768191	-4.285214
H	2.725918	-5.621285	-3.196922
H	2.218666	-1.799447	-5.108271
H	3.085818	-4.131134	-5.153020
C	0.675944	-3.148605	0.839088
C	0.101181	-4.399542	1.122334
C	1.690379	-2.659525	1.678418
C	0.525729	-5.139719	2.225824
H	-0.688930	-4.791120	0.488673
C	2.116469	-3.408093	2.776878
H	2.162480	-1.701461	1.487173
C	1.535118	-4.645245	3.055085
H	0.067717	-6.102559	2.436651
H	2.905570	-3.013394	3.410330
H	1.864518	-5.223027	3.914668
C	-4.965553	1.252991	2.454203
O	-5.066982	1.247868	3.665025
O	-5.981109	1.540261	1.611865
C	-7.239195	1.871085	2.240292
H	-7.093040	2.743074	2.886169
H	-7.546987	1.036510	2.878935
C	-8.241564	2.143228	1.134420
H	-9.213500	2.400952	1.569262
H	-7.912986	2.976471	0.505143
H	-8.370934	1.261768	0.498139
C	-3.699700	0.936696	1.744764
C	-3.560014	0.923110	0.438000
C	-3.419605	0.909735	-0.859073
H	-2.861882	0.715593	2.401671
H	-3.131283	1.807529	-1.402058
H	-3.604475	0.005849	-1.436258

IM6-b

Free Energy **=** -3696.299147810

Energy = -3696.88230681

Ni	-0.028903	0.582233	0.124603
C	-1.461036	-0.749729	0.506877
C	-1.524771	1.684369	-0.525170
C	-2.705374	-0.355338	-0.176084
C	-2.815435	1.120178	-0.081080
C	-3.575792	-1.091110	-0.912842
C	-3.899320	1.735899	0.448719
H	-4.430570	-0.601349	-1.368802
H	-4.752551	1.140203	0.758871
H	-1.240780	-1.813830	0.460959
H	-1.539808	-0.456815	1.569245
H	-1.428616	2.753372	-0.341987
H	-1.413292	1.485017	-1.602911
P	1.541148	-1.025033	0.670463
C	-4.023767	3.184383	0.667057
O	-3.176361	4.044327	0.487777
O	-5.270383	3.479683	1.132959
C	-3.448495	-2.526461	-1.180401
O	-2.498559	-3.254029	-0.925518
O	-4.566847	-2.991094	-1.804298
C	-4.565040	-4.390473	-2.140318
H	-3.702259	-4.604919	-2.780758
H	-4.444241	-4.979476	-1.224530
C	-5.878152	-4.693088	-2.839613
H	-6.728321	-4.472439	-2.186042
H	-5.981795	-4.094678	-3.750561
H	-5.920352	-5.752692	-3.115419
C	-5.526716	4.872025	1.393546
H	-4.805264	5.236960	2.132964
H	-5.366300	5.444360	0.473398
C	-6.956194	4.987784	1.891385
H	-7.662312	4.618936	1.140329
H	-7.098370	4.408055	2.809293
H	-7.194790	6.035791	2.104353
C	3.242029	-0.392835	1.022870
C	4.016255	0.093714	-0.046342
C	3.761692	-0.303977	2.322937
C	5.275326	0.646778	0.181801
H	3.638684	0.032344	-1.061439
C	5.022165	0.254347	2.547912
H	3.191309	-0.680047	3.165373
C	5.782117	0.731080	1.480360
H	5.860312	1.011264	-0.658185
H	5.409704	0.309117	3.561747
H	6.763530	1.162657	1.657198
C	1.091307	-1.965221	2.188833
C	1.148203	-3.363067	2.263866
C	0.647105	-1.242105	3.309484
C	0.777526	-4.022540	3.437541
H	1.473380	-3.940453	1.404827
C	0.287201	-1.902433	4.483597
H	0.577663	-0.157499	3.265477
C	0.350734	-3.296052	4.549066
H	0.820029	-5.107506	3.478616
H	-0.052618	-1.329408	5.341951
H	0.060893	-3.812269	5.460165
C	1.819528	-2.291920	-0.636839
C	3.041959	-2.977751	-0.750168
C	0.777325	-2.612494	-1.521299
C	3.218566	-3.951649	-1.732258
H	3.860228	-2.746001	-0.076028
C	0.957131	-3.593666	-2.497731

H	-0.186633	-2.125634	-1.438993
C	2.176584	-4.260494	-2.609644
H	4.170762	-4.469619	-1.810046
H	0.133910	-3.835101	-3.163533
H	2.315878	-5.020222	-3.374146
C	2.481309	2.785166	-2.666557
O	2.843251	2.737591	-3.826994
O	2.884381	3.734901	-1.793545
C	3.781245	4.731923	-2.327368
H	3.297386	5.225816	-3.176362
H	4.680506	4.234513	-2.706419
C	4.097958	5.705135	-1.207326
H	4.780275	6.481488	-1.570697
H	3.186857	6.189731	-0.842199
H	4.575206	5.191633	-0.366302
C	1.551252	1.796322	-2.068053
C	1.188567	1.788916	-0.792689
C	1.133345	2.205269	0.502972
H	1.190855	1.050831	-2.771776
H	0.503899	3.044594	0.788895
H	1.947814	1.959898	1.182346

TS7-b

Free Energy **=** -3696.268724790

Energy = -3696.84848579

Ni	1.078341	0.426138	-0.360017
C	-0.195645	0.358232	-1.927720
C	-0.224588	1.914859	-0.835131
C	-1.687746	0.497072	-1.793991
C	-1.706378	1.781727	-1.098865
C	-2.697311	-0.332348	-2.121450
C	-2.724364	2.615108	-0.810687
H	-3.725390	-0.056008	-1.907336
H	-3.740930	2.374418	-1.107650
P	0.314058	-0.972555	1.235663
C	-2.517417	3.876691	-0.079907
O	-1.451728	4.280921	0.354119
O	-3.684441	4.549368	0.063022
C	-2.485737	-1.658867	-2.724062
O	-1.409469	-2.205686	-2.912244
O	-3.668746	-2.229631	-3.048489
C	-3.594978	-3.543573	-3.643698
H	-2.973915	-3.489547	-4.543750
H	-3.097789	-4.221106	-2.941431
C	-5.013166	-3.984159	-3.954014
H	-5.618218	-4.027638	-3.042676
H	-5.493172	-3.292408	-4.653557
H	-5.001434	-4.980874	-4.408350
C	-3.601542	5.809214	0.765438
H	-3.200563	5.628655	1.768399
H	-2.893484	6.459422	0.241330
C	-4.997714	6.401437	0.806859
H	-5.380871	6.571117	-0.204464
H	-5.690688	5.734993	1.330571
H	-4.978419	7.361626	1.333769
C	0.757462	-0.507207	2.967456
C	1.516717	0.646814	3.203393
C	0.317875	-1.262997	4.068030
C	1.836559	1.035743	4.506409
H	1.856361	1.243446	2.363084
C	0.642835	-0.879081	5.367807
H	-0.287560	-2.150729	3.907800
C	1.403570	0.272253	5.589698
H	2.422124	1.936253	4.670280
H	0.297118	-1.474874	6.208481
H	1.652017	0.573573	6.603888
C	-1.492788	-1.336485	1.450082
C	-2.079097	-2.597562	1.278364
C	-2.320401	-0.252694	1.790974
C	-3.458285	-2.766882	1.430663
H	-1.463928	-3.455242	1.028109
C	-3.693877	-0.423486	1.949098
H	-1.887904	0.733988	1.938100
C	-4.269474	-1.683250	1.764380
H	-3.894780	-3.752899	1.293094
H	-4.315477	0.427386	2.215510
H	-5.341269	-1.817694	1.883481
C	1.080240	-2.627661	0.957940
C	2.016968	-3.186696	1.837989
C	0.790727	-3.303601	-0.242023
C	2.639963	-4.399522	1.534417
H	2.267737	-2.676134	2.761687
C	1.408140	-4.519001	-0.536020
H	0.081661	-2.888870	-0.954647
C	2.335563	-5.070831	0.350689
H	3.366040	-4.816651	2.227368
H	1.169107	-5.027984	-1.465852
H	2.821927	-6.013865	0.116016
C	4.421716	2.141725	-2.522787
O	4.727710	2.866187	-3.454967
O	5.344258	1.523841	-1.739584
C	6.716846	1.777814	-2.087058
H	6.909199	2.855075	-2.031813
H	6.888674	1.470908	-3.124640
C	7.584737	0.998146	-1.115586
H	8.644025	1.164173	-1.342132
H	7.398154	1.315740	-0.084401
H	7.380503	-0.075343	-1.185061
C	3.027417	1.850636	-2.136121
C	2.638586	1.058067	-1.133205
C	3.008801	0.225505	-0.070694
H	2.305433	2.360997	-2.771914
H	3.444284	0.670413	0.825588
H	3.394743	-0.773635	-0.282854
H	0.187648	-0.673995	-1.895741
H	0.166595	0.808825	-2.856406
H	0.247955	2.712312	-1.410842
H	0.014108	2.087788	0.229649

IM7-b

Free Energy **=** -3696.297377490

Energy = -3696.88474549

Ni	0.314992	0.005782	-0.823131
P	-1.418458	-0.367007	0.650861
C	-1.516301	0.928808	1.971446
C	-0.533862	1.924769	2.058215
C	-2.578901	0.950199	2.893095
C	-0.601722	2.908430	3.048208

H	0.283355	1.945043	1.345401
C	-2.644848	1.931067	3.881181
H	-3.365203	0.203717	2.831017
C	-1.653976	2.912877	3.962396
H	0.169175	3.672775	3.096430
H	-3.473975	1.932426	4.583881
H	-1.708204	3.680146	4.730182
C	-3.205592	-0.466251	0.171146
C	-3.937651	-1.661614	0.172753
C	-3.845470	0.720720	-0.231976
C	-5.280052	-1.671762	-0.216077
H	-3.470204	-2.588595	0.488028
C	-5.186527	0.705978	-0.612438
H	-3.291081	1.654597	-0.268283
C	-5.908897	-0.490132	-0.606116
H	-5.832927	-2.607505	-0.205571
H	-5.664726	1.631879	-0.920623
H	-6.953756	-0.499276	-0.904820
C	-1.134197	-1.948737	1.569544
C	-1.096496	-2.047631	2.967665
C	-0.898658	-3.105817	0.806054
C	-0.842027	-3.274402	3.586182
H	-1.257846	-1.168315	3.581619
C	-0.658140	-4.331639	1.426327
H	-0.884115	-3.059025	-0.278864
C	-0.628172	-4.419806	2.819792
H	-0.810754	-3.330029	4.671275
H	-0.482895	-5.211492	0.813253
H	-0.431709	-5.372713	3.304113
C	-1.489245	-1.413802	-3.056400
C	-0.099547	-0.899100	-2.699712
C	-0.545867	0.466205	-2.652235
C	-1.962183	0.082429	-3.062246
H	-1.530044	-1.919924	-4.026355
H	-1.968219	-2.053498	-2.312677
H	-2.204667	0.462607	-4.060941
H	-2.770434	0.345903	-2.384185
C	0.177808	1.601377	-2.281258
C	1.147461	-1.401600	-2.363864
C	1.337640	-2.842844	-2.153408
O	0.464249	-3.697052	-2.179798
O	2.638911	-3.127030	-1.889869
C	-0.516832	2.868801	-2.009195
O	-1.714423	3.010776	-1.815790
O	0.362159	3.903464	-1.979412
C	2.944487	-4.516888	-1.647600
H	2.351214	-4.866754	-0.796154
H	2.642498	-5.102670	-2.522101
C	4.435021	-4.617112	-1.382152
H	4.710638	-5.660916	-1.195608
H	5.010025	-4.256688	-2.241089
H	4.717054	-4.023953	-0.506256
C	-0.191323	5.197534	-1.661052
H	-0.675885	5.143455	-0.680200
H	-0.964656	5.442647	-2.396535
C	0.950122	6.197393	-1.678746
H	1.418925	6.237484	-2.667233
H	0.573472	7.197007	-1.434991
H	1.717818	5.928406	-0.946201
H	1.225056	1.685280	-2.548090
H	2.047076	-0.815463	-2.518877
C	3.963767	2.041631	0.523293
O	4.634408	3.051910	0.404206
O	4.286831	1.035930	1.373792
C	5.492056	1.233493	2.138256
H	5.393275	2.148572	2.732300
H	6.331591	1.380919	1.450438
C	5.683561	0.007891	3.012690
H	6.592570	0.116532	3.614761
H	4.834260	-0.125116	3.690818
H	5.780011	-0.895958	2.402339
C	2.720121	1.799213	-0.241763
C	1.945363	0.720632	-0.110097
C	1.668471	-0.450030	0.570415
H	1.325016	-0.400863	1.602740
H	2.166580	-1.380849	0.306448
H	2.475353	2.607755	-0.923618

TS8-b

Free Energy **=** -3696.291067630

Energy = -3696.87139163

C	-2.564229	0.646433	-2.617879
C	-2.295580	1.634006	-1.492817
C	-3.601205	1.341761	-0.868582
C	-3.912363	0.282704	-1.914729
H	-2.663542	1.126669	-3.597596
H	-1.843232	-0.167840	-2.703172
H	-4.831818	0.452759	-2.482152
H	-3.940535	-0.733138	-1.509886
C	-4.241088	1.824872	0.211232
C	-1.272630	2.441916	-1.156991
C	-0.012866	2.469466	-1.924097
O	0.358828	1.615995	-2.715312
O	0.706385	3.574684	-1.629257
C	-5.550479	1.292765	0.629966
O	-6.155371	0.381089	0.092399
O	-6.013254	1.953597	1.719670
C	1.959512	3.728480	-2.336804
H	2.630486	2.913910	-2.048639
H	1.768264	3.641773	-3.410941
C	2.524975	5.085811	-1.964537
H	3.476913	5.244563	-2.482589
H	1.837626	5.888915	-2.249492
H	2.706319	5.150210	-0.887033
C	-7.291113	1.510306	2.225412
H	-7.222039	0.446832	2.477154
H	-8.039382	1.611293	1.432317
C	-7.624408	2.362633	3.435662
H	-7.686049	3.421380	3.163927
H	-8.590686	2.056443	3.851053
H	-6.863415	2.250601	4.214746
H	-3.811254	2.620302	0.813834
H	-1.347163	3.116751	-0.308143
Ni	0.924457	-1.031514	-0.891214
P	2.529365	-0.418376	0.445843
C	3.519968	-1.898732	0.922720
C	2.897663	-3.152277	0.820289
C	4.844914	-1.832572	1.380941
C	3.577028	-4.314651	1.184433

H	1.884311	-3.200887	0.434082
C	5.524566	-2.996679	1.742091
H	5.352162	-0.874009	1.442504
C	4.891326	-4.238126	1.648124
H	3.082477	-5.278088	1.096241
H	6.551306	-2.934328	2.093165
H	5.424582	-5.143021	1.927074
C	3.832263	0.765413	-0.114206
C	4.111891	1.979470	0.527049
C	4.537600	0.441810	-1.286517
C	5.080760	2.846063	0.012498
H	3.578330	2.250076	1.432581
C	5.504252	1.305412	-1.797719
H	4.333823	-0.496262	-1.798731
C	5.779406	2.512305	-1.147872
H	5.291078	3.781088	0.525327
H	6.042960	1.037416	-2.702664
H	6.533925	3.186044	-1.544912
C	1.922525	0.291551	2.031803
C	2.601440	0.169395	3.253015
C	0.716845	1.007424	1.992170
C	2.088114	0.762832	4.406950
H	3.525660	-0.397719	3.307889
C	0.207895	1.605990	3.144841
H	0.169890	1.065457	1.055514
C	0.894059	1.485427	4.354275
H	2.620029	0.657442	5.348816
H	-0.728983	2.154692	3.100146
H	0.495630	1.944170	5.255282
C	-2.396156	-3.523927	-2.117822
O	-2.840235	-4.295342	-2.951075
O	-3.047828	-3.249904	-0.951387
C	-4.280603	-3.966651	-0.744259
H	-4.057536	-5.035744	-0.647900
H	-4.919048	-3.845649	-1.625044
C	-4.933036	-3.410919	0.509371
H	-5.854971	-3.964076	0.723086
H	-4.265659	-3.509704	1.372280
H	-5.190787	-2.353535	0.387450
C	-1.134987	-2.773797	-2.276076
C	-0.515556	-2.064967	-1.320557

IM-DPPE

Free Energy = -3964.0586818

Energy = -3964.66545883

Ni	0.000105	-0.246894	0.000191
C	-1.064809	1.197350	0.834615
C	1.064959	1.196957	-0.834989
C	-0.735289	2.436381	0.120423
C	0.735482	2.436326	-0.121356
C	-1.543241	3.386192	-0.419248
C	1.543394	3.386422	0.417864
H	-1.100544	4.226029	-0.945966
H	1.100658	4.226490	0.944181
H	-2.127591	1.060929	1.021852
H	-0.523999	1.182075	1.796631
H	2.127720	1.060428	-1.022297
H	0.524018	1.181263	-1.796930
C	-0.555000	-1.704630	0.044683
H	-0.366670	-2.461046	0.813042
H	-1.269739	-0.945778	0.379890
H	-0.720959	-2.858772	-3.278836

2

Free Energy = -767.812528270

Energy = -768.028413270

C	0.782561	2.341550	0.000449
C	-0.782528	2.341556	0.000330
C	0.737113	0.820111	0.000281
C	-0.737093	0.820115	0.000000
C	1.664751	-0.153250	0.000350
C	-1.664740	-0.153245	-0.000747
H	1.380755	-1.201843	0.000268
H	-1.380748	-1.201838	-0.001125
C	-3.105812	0.159012	-0.000821
O	-3.591275	1.276550	-0.001098
O	-3.844780	-0.977235	-0.000588
C	3.105823	0.159019	0.000427
O	3.591265	1.276562	0.000989
O	3.844773	-0.977236	-0.000377
C	5.277033	-0.793334	-0.000373
H	5.558146	-0.209211	-0.883016
H	5.558152	-0.209077	0.882167
C	5.915099	-2.169826	-0.000299
H	5.619535	-2.738444	0.887327
H	5.619423	-2.738602	-0.887787
H	7.006324	-2.073496	-0.000378
C	-5.277046	-0.793322	-0.000452
H	-5.557923	-0.207808	0.881326
H	-5.558394	-0.210452	-0.883853
C	-5.915131	-2.169802	0.001713
H	-5.619658	-2.739839	-0.885033
H	-5.619375	-2.737164	0.890078
H	-7.006358	-2.073468	0.001737
H	-1.261062	2.775053	0.883524
H	-1.260940	2.775259	-0.882809
H	1.261007	2.775060	0.883664
H	1.261077	2.775242	-0.882663
C	3.005117	3.361763	0.381170
O	3.737673	2.445926	0.026113
O	3.511551	4.543605	0.839654
C	-3.004966	3.361427	-0.382668
O	-3.737499	2.445784	-0.027077
O	-3.511449	4.542937	-0.841988
C	-4.945030	4.639837	-0.879731
H	-5.343507	3.847166	-1.523440
H	-5.345135	4.471594	0.126175
C	-5.295476	6.021227	-1.403693
H	-4.890277	6.800268	-0.749754
H	-4.888351	6.172664	-2.408828
H	-6.383826	6.140582	-1.450000
C	4.945126	4.640591	0.877375
H	5.343654	3.848034	1.521187
H	5.345230	4.472239	-0.128515
C	5.295491	6.022081	1.401133
H	4.890206	6.801006	0.747109

H	4.888399	6.173617	2.406266
H	6.383835	6.141522	1.447373
C	0.530690	-3.435505	-0.552676
C	-0.530674	-3.434884	0.555934
P	1.433227	-1.796449	-0.532527
P	-1.433136	-1.795865	0.533919
C	2.292581	-1.802046	-2.156321
C	1.500392	-1.627606	-3.303247
C	3.674911	-1.972459	-2.303683
C	2.078718	-1.637427	-4.571152
H	0.428146	-1.472443	-3.203164
C	4.252887	-1.975102	-3.574982
H	4.303319	-2.097930	-1.427806
C	3.458039	-1.810846	-4.709356
H	1.454701	-1.500052	-5.450125
H	5.327235	-2.104072	-3.675810
H	3.910729	-1.810817	-5.697254
C	2.754175	-1.967471	0.737209
C	3.026547	-3.170650	1.406996
C	3.506854	-0.824114	1.066119
C	4.022705	-3.232528	2.383434
H	2.467637	-4.071898	1.176026
C	4.509346	-0.895212	2.033357
H	3.321492	0.127471	0.576589
C	4.768169	-2.095849	2.697278
H	4.216001	-4.172101	2.894491
H	5.081688	-0.001739	2.266184
H	5.544637	-2.145582	3.456098
C	-2.293343	-1.799947	2.157256
C	-1.501934	-1.623527	3.304415
C	-3.675610	-1.971431	2.304067
C	-2.080952	-1.632398	4.572019
H	-0.429772	-1.467541	3.204753
C	-4.254277	-1.973127	3.575042
H	-4.303424	-2.098465	1.427986
C	-3.460189	-1.806863	4.709663
H	-1.457539	-1.493473	5.451177
H	-5.328565	-2.102934	3.675449
H	-3.913429	-1.806097	5.697309
C	-2.753495	-1.967957	-0.736292
C	-3.025002	-3.171534	-1.405723
C	-3.506530	-0.825069	-1.066025
C	-4.020657	-3.234253	-2.382625
H	-2.465841	-4.072454	-1.174078
C	-4.508510	-0.897008	-2.033722
H	-3.321826	0.126766	-0.576712
C	-4.766466	-2.098032	-2.697295
H	-4.213299	-4.174123	-2.893381
H	-5.081170	-0.003911	-2.267212
H	-5.542535	-2.148400	-3.456481
H	0.052936	-3.490657	-1.537759
H	1.207103	-4.293822	-0.479985
H	-1.207106	-4.293276	0.484234
H	-0.052912	-3.488914	1.541086

TS-DPPE

Free Energy = -3963.9941017

Energy = -3964.59330772

C	1.111869	-2.381557	1.932325
C	2.499993	-1.948290	1.433044
P	-0.207465	-1.085741	1.558001
P	2.394412	-1.044480	-0.221010
C	-0.129703	0.067930	3.000540
C	0.872705	0.038261	3.980476
C	-1.116032	1.067223	3.085695
C	0.891179	0.979996	5.013562
H	1.650845	-0.717706	3.949871
C	-1.104331	1.999144	4.120663
H	-1.897320	1.111292	2.330536
C	-0.096408	1.960627	5.088547
H	1.680440	0.942294	5.760134
H	-1.879200	2.759758	4.169842
H	-0.081251	2.692217	5.891986
C	-1.725098	-2.081108	1.928938
C	-2.113261	-2.410921	3.237900
C	-2.491783	-2.558893	0.857058
C	-3.237141	-3.204170	3.467516
H	-1.540401	-2.038349	4.082953
C	-3.613531	-3.358744	1.087413
H	-2.231203	-2.298192	-0.164115
C	-3.988769	-3.683027	2.391289
H	-3.526654	-3.448722	4.486602
H	-4.192691	-3.719740	0.241482
H	-4.864907	-4.301007	2.571024
C	2.681795	-2.360987	-1.479869
C	3.066907	-1.974774	-2.776428
C	2.433879	-3.720109	-1.236608
C	3.211937	-2.918595	-3.790653
H	3.264058	-0.926461	-2.986681
C	2.572804	-4.665723	-2.255616
H	2.130523	-4.054598	-0.249418
C	2.963177	-4.269887	-3.534321
H	3.518039	-2.599355	-4.783609
H	2.376038	-5.713942	-2.045415
H	3.070935	-5.006016	-4.326330
C	4.005660	-0.136440	-0.216291
C	3.991206	1.253995	-0.033631
C	5.244221	-0.786119	-0.348668
C	5.184304	1.978379	0.021404
H	3.042876	1.776922	0.056949
C	6.435495	-0.063318	-0.295722
H	5.276479	-1.861070	-0.504888
C	6.407761	1.321410	-0.109183
H	5.153196	3.055930	0.158850
H	7.386171	-0.580029	-0.401446
H	7.336690	1.884565	-0.071193
H	1.131916	-2.646468	2.996399
H	0.771778	-3.274036	1.393704
H	2.934810	-1.212603	2.119086
H	3.193895	-2.796322	1.389384
Ni	0.439529	-0.134377	-0.281082
C	-0.776001	0.049507	-1.897009
C	0.222244	1.534612	-1.233208
C	-1.922574	0.989883	-1.668224
C	-1.131143	2.186502	-1.377226
C	-3.262974	0.818386	-1.687548
C	-1.486933	3.487197	-1.319866
H	-3.922020	1.644660	-1.436986
H	-2.521014	3.787650	-1.460157

C	-0.509980	4.551018	-1.055501
O	0.686655	4.399725	-0.866043
O	-1.113421	5.768008	-1.039282
C	-3.908822	-0.456205	-2.015677
O	-3.352809	-1.519192	-2.251529
O	-5.260725	-0.317866	-2.025886
C	-6.013867	-1.508943	-2.326185
H	-5.682940	-1.908005	-3.290727
H	-5.796194	-2.267166	-1.565689
C	-7.483201	-1.128873	-2.339946
H	-7.792157	-0.728350	-1.369005
H	-7.683372	-0.370722	-3.103968
H	-8.095002	-2.010679	-2.560226
C	-0.249595	6.893693	-0.783909
H	0.253742	6.745581	0.177473
H	0.525855	6.929610	-1.556733
C	-1.113714	8.141417	-0.787855
H	-1.611892	8.268683	-1.754421
H	-1.882058	8.086919	-0.009834
H	-0.494236	9.025270	-0.599870
H	-0.944353	-1.016638	-1.683961
H	-0.399240	0.119503	-2.923477
H	0.983634	1.883150	-1.932397
H	0.633934	1.637674	-0.181732

TS3-b'

Free Energy = -3312.37615434

Energy = -3312.84099534

Ni	-0.096627	-0.888765	-1.235021
C	-1.855699	-1.618930	-1.683983
C	1.771333	-1.342686	-1.535490
C	-0.820820	-2.625501	-1.568084
C	0.852736	-2.090598	-2.375216
C	-0.729830	-3.885271	-1.141488
C	0.900795	-2.550337	-3.626082
H	0.226436	-4.363565	-0.964383
H	0.029459	-2.942506	-4.141056
H	-2.152761	-1.343396	-2.696962
P	-0.107021	0.978634	-0.113990
C	2.488719	-2.029129	-0.449430
O	2.261888	-3.141106	-0.002743
O	3.480209	-1.235715	0.058506
C	-3.011607	-1.550901	-0.776076
O	-4.092662	-1.076841	-1.083897
O	-2.765994	-2.040400	0.475431
C	-3.879447	-1.972768	1.389036
H	-4.181393	-0.927029	1.508133
H	-4.729118	-2.510484	0.955441
C	-3.435988	-2.587251	2.704314
H	-3.116079	-3.624910	2.563509
H	-2.603171	-2.025093	3.139765
H	-4.266657	-2.576205	3.418978
C	4.209925	-1.788848	1.171948
H	3.502615	-2.063137	1.960957
H	4.713509	-2.705788	0.847356
C	5.198672	-0.736954	1.641018
H	5.883861	-0.454972	0.834605
H	4.676519	0.162393	1.984101
H	5.792299	-1.128125	2.474912
C	1.037064	2.252862	-0.797085
C	2.423945	2.022067	-0.765655
C	0.553880	3.413375	-1.417846
C	3.302385	2.943172	-1.335166
H	2.818026	1.124379	-0.298913
C	1.438668	4.327726	-1.993632
H	-0.513005	3.608452	-1.452451
C	2.813362	4.097174	-1.952121
H	4.372164	2.754968	-1.299300
H	1.048821	5.222498	-2.471599
H	3.500706	4.810820	-2.398515
C	-1.693671	1.886468	0.109218
C	-1.949256	2.683994	1.236584
C	-2.664699	1.798678	-0.898032
C	-3.150477	3.382848	1.346609
H	-1.214843	2.752717	2.033179
C	-3.864941	2.502830	-0.787372
H	-2.494901	1.158570	-1.757306
C	-4.108852	3.296008	0.333401
H	-3.339577	3.993055	2.225904
H	-4.613243	2.410657	-1.568860
H	-5.047025	3.836990	0.424377
C	0.488955	0.652299	1.595838
C	1.253193	1.567425	2.334961
C	0.134566	-0.573801	2.182593
C	1.656111	1.261016	3.636433
H	1.545511	2.514967	1.892785
C	0.538018	-0.875163	3.483969
H	-0.457244	-1.292905	1.622208
C	1.299892	0.040322	4.212849
H	2.249172	1.977683	4.198526
H	0.263354	-1.830492	3.922644
H	1.618028	-0.197621	5.224379
H	-1.635442	-4.453967	-0.941559
H	1.847133	-2.578728	-4.162599
H	2.338612	-0.551580	-2.022250

IM4-b'

Free Energy = -3312.40309973

Energy = -3312.86973873

Ni	-0.358185	-0.724992	-0.027304
C	-1.958803	-1.820525	0.140757
C	-1.090809	-0.012566	-1.665106
C	-2.508644	-1.970157	-1.247870
C	-2.392197	-0.707103	-2.011323
C	-2.922196	-3.133335	-1.775293
C	-3.299773	-0.266953	-2.891361
H	-3.212668	-3.211584	-2.819629
H	-4.219156	-0.816969	-3.072186
H	-1.659309	-2.774502	0.588537
H	-0.319725	-0.315242	-2.386928
H	-3.170853	0.666500	-3.432440
C	-1.043692	1.475732	-1.612830
O	-0.067678	2.153424	-1.913503
O	-2.179826	2.044576	-1.137521
C	-2.170023	3.481117	-1.031550
C	-3.555817	3.918487	-0.593463
H	-1.892858	3.910087	-1.999841
H	-1.404059	3.782194	-0.307870

H	-3.592588	5.010059	-0.503237
H	-4.311011	3.606475	-1.321997
H	-3.814643	3.483587	0.377297
H	-2.967335	-4.042844	-1.180711
C	-2.801919	-1.091031	1.133606
O	-2.552594	-0.982103	2.329512
O	-3.909834	-0.533735	0.589912
C	-4.731793	0.249125	1.473439
C	-5.938245	0.710060	0.675529
H	-4.145864	1.094451	1.852263
H	-5.018293	-0.362527	2.335359
H	-6.593302	1.324338	1.304026
H	-5.624420	1.302927	-0.188955
H	-6.513487	-0.147481	0.311527
P	1.674893	0.075190	0.061096
C	2.997300	-0.269229	-1.150661
C	2.712299	-1.134780	-2.219958
C	4.269075	0.315236	-1.062365
C	3.690001	-1.424657	-3.170581
H	1.724377	-1.578241	-2.308993
C	5.241223	0.029772	-2.021515
H	4.498163	0.996942	-0.249264
C	4.955185	-0.841304	-3.073962
H	3.458861	-2.096243	-3.992662
H	6.222615	0.490040	-1.945594
H	5.713448	-1.060237	-3.820845
C	2.216241	1.486605	1.085799
C	2.946182	1.317247	2.273174
C	1.878535	2.781762	0.656974
C	3.331190	2.428751	3.023331
H	3.204675	0.319285	2.615077
C	2.275024	3.887947	1.409647
H	1.303692	2.913067	-0.256131
C	2.998239	3.714365	2.591383
H	3.891714	2.289960	3.943912
H	2.012108	4.887440	1.073883
H	3.299421	4.578707	3.177272
C	1.521909	-1.380470	1.150822
C	2.197398	-2.606844	0.959710
C	0.473587	-1.313047	2.097249
C	1.848537	-3.718598	1.711726
H	2.994329	-2.672543	0.225610
C	0.131986	-2.450623	2.849207
H	-0.007640	-0.371548	2.350890
C	0.810860	-3.644574	2.657051
H	2.384950	-4.653108	1.568921
H	-0.685010	-2.376926	3.557539
H	0.543946	-4.523899	3.236641

TS4-b'

Free Energy = -3312.34449815

Energy = -3312.81124915

Ni	-0.732220	-0.162579	-0.281642
C	-2.474240	0.608934	-1.610502
C	-1.890407	1.685728	-0.470936
C	-3.823311	1.297559	-1.450966
C	-3.311337	2.247286	-0.449625
C	-5.003570	1.099959	-2.041001
C	-3.825532	3.257797	0.254300
H	-5.863008	1.724120	-1.810846
H	-4.864827	3.556678	0.145935
H	-1.991573	0.801479	-2.572341
H	-1.163760	2.386846	-0.884407
H	-3.217510	3.806466	0.967932
C	-1.356521	1.261635	0.910237
O	-0.727350	2.040122	1.634214
O	-2.153747	0.223567	1.449115
C	-2.040005	0.036289	2.875404
C	-3.039241	-1.028968	3.287108
H	-2.241094	0.997343	3.359365
H	-1.015773	-0.256541	3.125372
H	-2.993483	-1.182999	4.371334
H	-4.059013	-0.731997	3.021821
H	-2.818128	-1.984019	2.798182
H	-5.153646	0.299169	-2.759045
C	-2.343752	-0.864138	-1.298362
O	-1.341905	-1.543152	-1.661559
O	-3.437024	-1.429661	-0.748540
C	-3.359643	-2.844155	-0.475844
C	-4.725349	-3.283594	0.017964
H	-2.581998	-3.021122	0.275119
H	-3.065508	-3.367228	-1.391475
H	-4.715742	-4.358161	0.231419
H	-4.999299	-2.750363	0.933531
H	-5.493478	-3.088021	-0.737079
P	1.401113	-0.070606	-0.081177
C	2.127517	1.587348	-0.466348
C	1.755246	2.170707	-1.689665
C	3.013394	2.282324	0.365733
C	2.252372	3.416009	-2.068861
H	1.075446	1.639944	-2.353076
C	3.506272	3.534532	-0.011471
H	3.319669	1.852468	1.313567
C	3.128446	4.104938	-1.226271
H	1.954805	3.849708	-3.020107
H	4.188703	4.062577	0.649611
H	3.512142	5.079581	-1.515945
C	2.090678	-0.518264	1.576399
C	2.901150	-1.647028	1.768516
C	1.733443	0.257068	2.696269
C	3.347982	-1.992809	3.045962
H	3.186640	-2.262308	0.921876
C	2.192810	-0.087541	3.968000
H	1.085110	1.119822	2.570481
C	3.000370	-1.212972	4.148561
H	3.973928	-2.872293	3.174489
H	1.914751	0.526499	4.821038
H	3.353984	-1.479891	5.141132
C	2.347841	-1.165136	-1.233231
C	3.660871	-0.872047	-1.636464
C	1.746192	-2.346387	-1.692780
C	4.354350	-1.739872	-2.479775
H	4.141395	0.039701	-1.294588
C	2.444691	-3.216439	-2.532706
H	0.722393	-2.569637	-1.412986
C	3.748265	-2.915608	-2.928563
H	5.368557	-1.497149	-2.786626
H	1.963342	-4.125201	-2.884641
H	4.288737	-3.590122	-3.587761

TS7-b'

Free Energy = -3696.22141685

Energy = -3696.80773985

Ni	-0.606832	-0.575345	-0.136055
C	-0.339436	-2.778046	-0.596794
C	-0.662922	-2.418449	1.116305
C	0.355645	-4.004837	-0.009525
C	0.308663	-3.553640	1.381611
C	0.753785	-5.127911	-0.609070
C	0.929115	-3.936737	2.499152
H	0.675621	-5.262110	-1.684300
H	0.804043	-3.398237	3.432511
P	1.157676	0.946650	-0.022248
C	-0.567542	-1.215330	2.042638
O	0.469906	-0.823458	2.568838
O	-1.795156	-0.868482	2.510316
C	0.453080	-2.029344	-1.656200
O	-0.062562	-1.564805	-2.666866
O	1.785516	-2.146972	-1.491495
C	2.618777	-1.741903	-2.606426
H	2.123602	-2.043065	-3.533498
H	2.699070	-0.651117	-2.602508
C	3.970999	-2.406746	-2.433090
H	4.447602	-2.090906	-1.501519
H	3.867759	-3.496697	-2.422193
H	4.624156	-2.129712	-3.268244
C	-1.819983	0.118474	3.566251
H	-1.192530	-0.234800	4.391105
H	-1.386119	1.050276	3.191821
C	-3.268184	0.294589	3.982946
H	-3.877586	0.639680	3.141762
H	-3.689108	-0.647854	4.347764
H	-3.334176	1.036641	4.786372
C	0.875712	2.146839	1.365741
C	-0.138525	3.112869	1.250609
C	1.602256	2.078875	2.561995
C	-0.416010	3.986420	2.302708
H	-0.701890	3.199112	0.327450
C	1.324406	2.954147	3.613497
H	2.385469	1.339239	2.679955
C	0.314457	3.908760	3.490314
H	-1.200255	4.730571	2.189959
H	1.902026	2.886233	4.531672
H	0.100925	4.589990	4.309790
C	2.939705	0.466832	0.210362
C	4.002578	1.133607	-0.419580
C	3.233042	-0.611708	1.062200
C	5.324023	0.743786	-0.191420
H	3.806802	1.958976	-1.095184
C	4.556021	-0.990025	1.297829
H	2.424485	-1.139991	1.554671
C	5.606103	-0.314826	0.673075
H	6.132502	1.273145	-0.689276
H	4.762414	-1.820722	1.967725
H	6.635389	-0.613493	0.854565
C	1.217567	2.081410	-1.487701
C	1.711622	3.394907	-1.396182
C	0.783180	1.614367	-2.738369
C	1.772330	4.214819	-2.523070
H	2.043064	3.783506	-0.438325
C	0.845716	2.437936	-3.865615
H	0.392623	0.606869	-2.840155
C	1.339145	3.737965	-3.762191
H	2.156006	5.227626	-2.430938
H	0.500270	2.058397	-4.823518
H	1.382517	4.378782	-4.638967
C	-4.865670	-0.993990	-1.024988
O	-5.779862	-1.788539	-1.163511
O	-5.026516	0.346329	-1.173916
C	-6.356237	0.773006	-1.521549
H	-7.056042	0.436095	-0.748866
H	-6.653820	0.293136	-2.460275
C	-6.332050	2.286063	-1.642722
H	-7.328588	2.657348	-1.907052
H	-6.031279	2.748583	-0.696794
H	-5.627932	2.604157	-2.418549
C	-3.485538	-1.389761	-0.679338
C	-2.454038	-0.559126	-0.521720
C	-1.993937	0.752994	-0.540423
H	-3.387541	-2.467055	-0.555973
H	-2.249370	1.410078	0.291918
H	-1.863937	1.266640	-1.493909
H	-1.307152	-2.992095	-1.045750
H	-1.693877	-2.771533	1.166353
H	1.610325	-4.783436	2.498356
H	1.172957	-5.952629	-0.039201