SUPPLEMENTARY INFORMATION

Mechanistic Study of the Cooperative Palladium/Lewis Acid-Catalyzed Transfer Hydrocyanation Reaction: The Origin of the Regioselectivity

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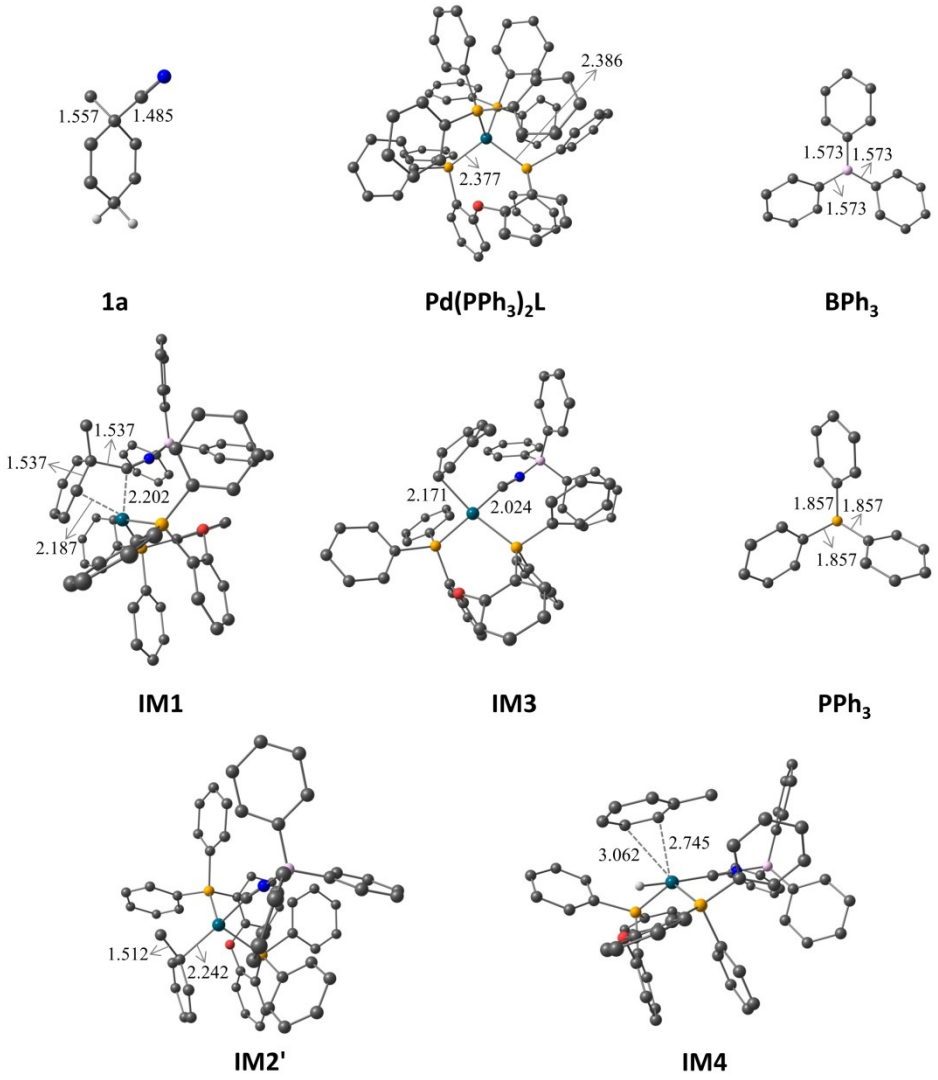

Fig. S1 Optimized geometries according to the reaction pathway in Fig. 1. Key bond distances are given in Å. Some hydrogen atoms are omitted for clarity (color code, C: black, O: red, H: white, N: blue, P: orange, Pd: green, B: pink).

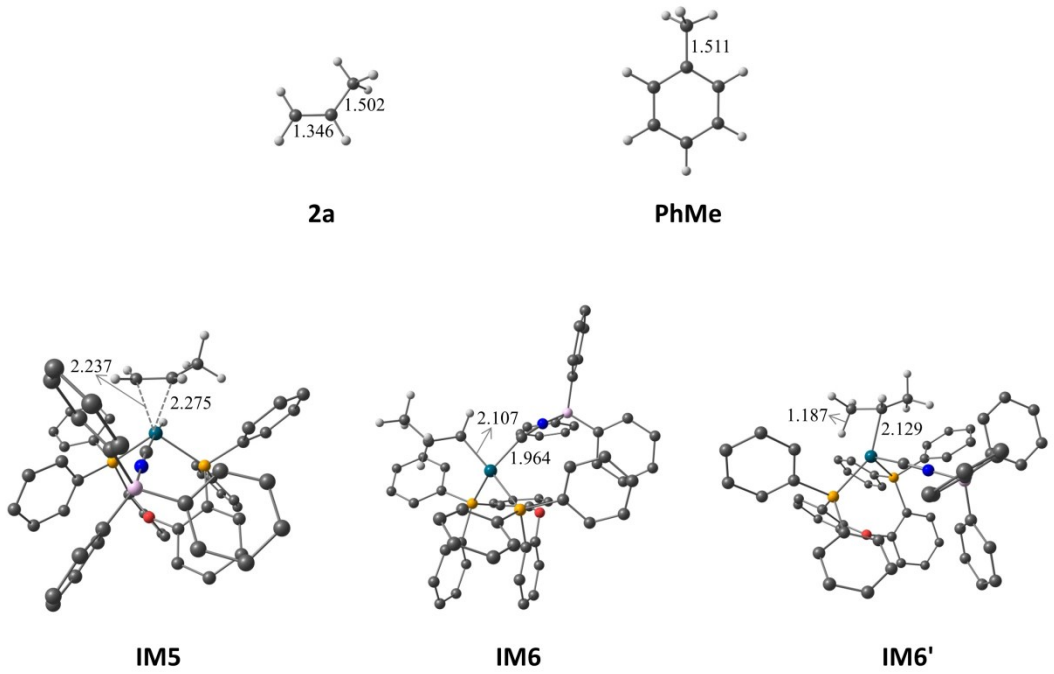

Fig. S2 Optimized geometries according to the reaction pathway in Fig. 2. Key bond distances are given in Å. Some hydrogen atoms are omitted for clarity (color code, C: black, O: red, H: white, N: blue, P: orange, Pd: green, B: pink).

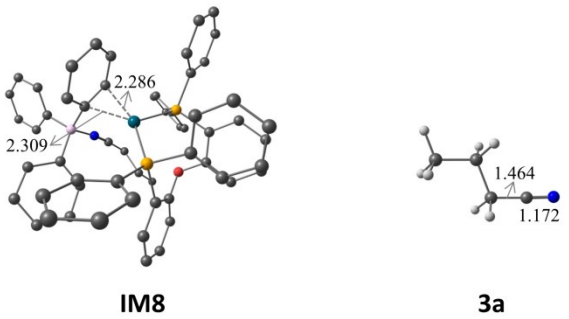

Fig. S3 Optimized geometries according to the reaction pathway in Fig. 3. Key bond distances are given in Å. Some hydrogen atoms are omitted for clarity (color code, C: black, O: red, H: white, N: blue, P: orange, Pd: green, B: pink).

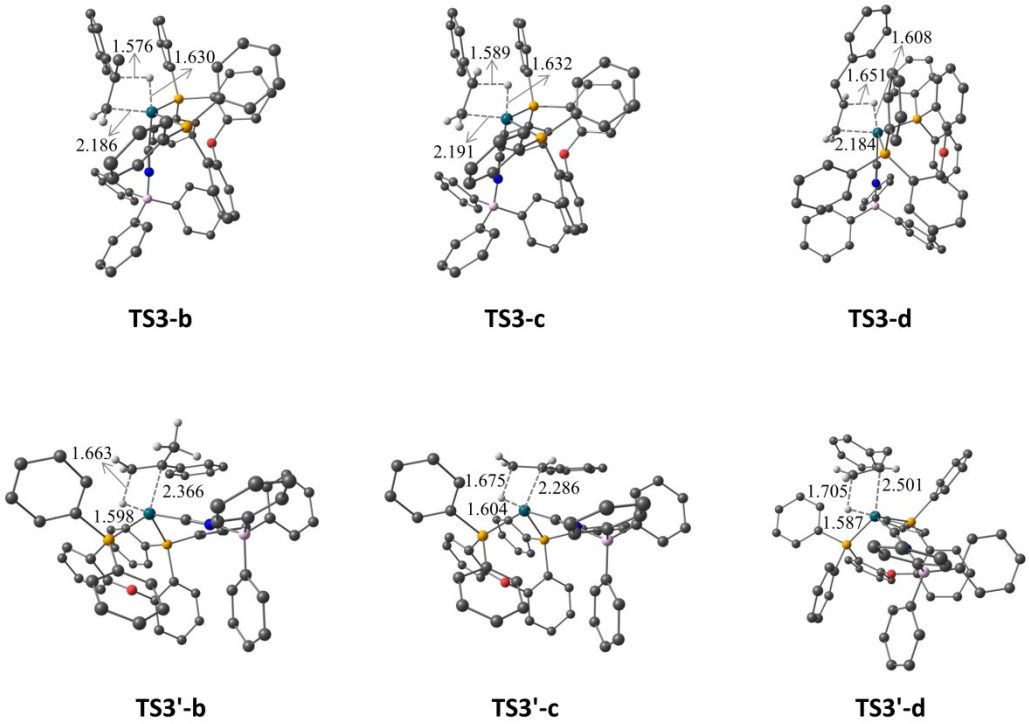

Fig. S4 Optimized geometries of the structure according to Table 1. Key bond distances are given in Å. Some hydrogen atoms are omitted for clarity (color code, C: black, O: red, H: white, N: blue, P: orange, Pd: green, B: pink).

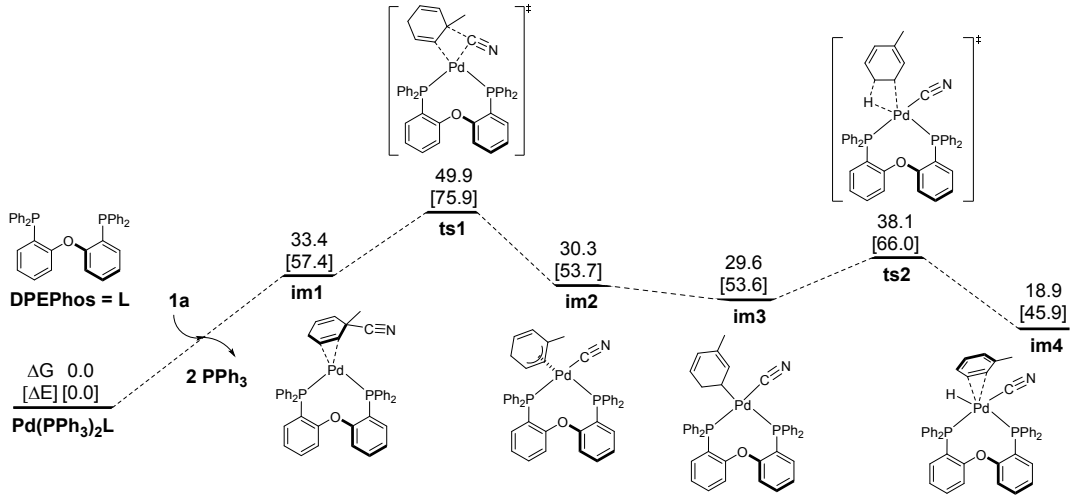

Fig. S5 Computed free energy profile (in kcal mol^{-1}) for the stage I without Lewis acid binding to the N atom of nitrile at the BP86+D3/def2-TZVPP (smd, solvent=1,4 Dioxane)//BP86+D3/def2-SVP (smd, solvent = 1,4-Dioxane) level.

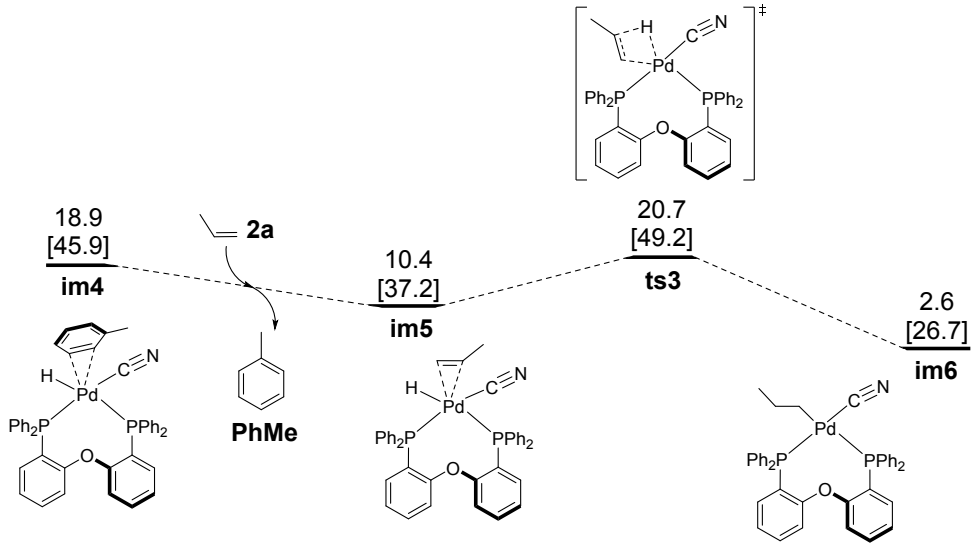

Fig. S6 Computed free energy profile (in kcal mol^{-1}) for the stage II without Lewis acid binding to the N atom of nitrile at the BP86+D3/def2-TZVPP (smd, solvent=1,4 Dioxane)//BP86+D3/def2-SVP (smd, solvent = 1,4-Dioxane) level.

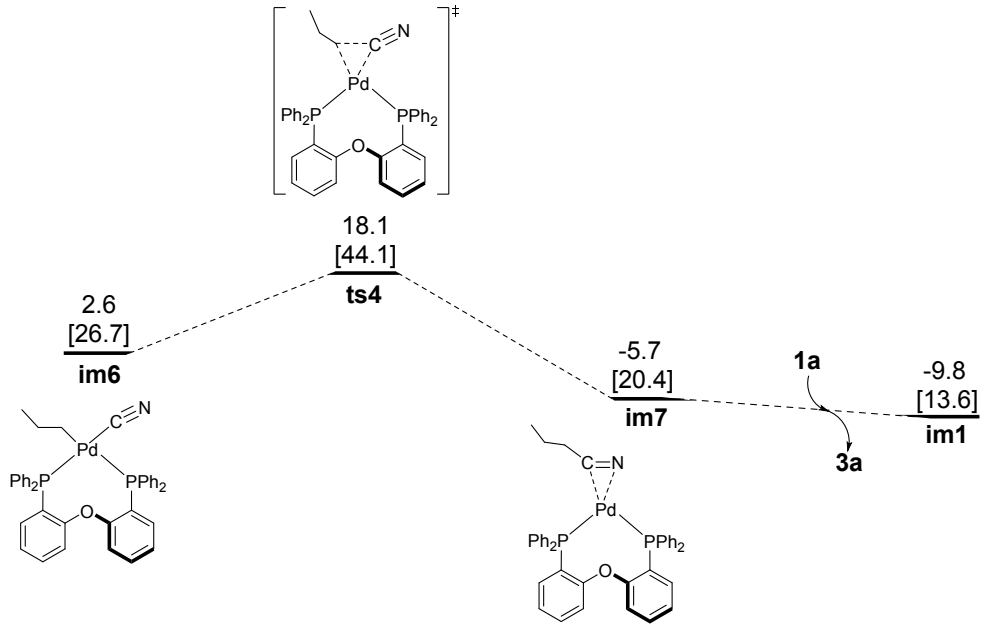

Fig. S7 Computed free energy profile (in kcal mol^{-1}) for the stage III without Lewis acid binding to the N atom of nitrile at the BP86+D3/def2-TZVPP (smd, solvent=1,4 Dioxane)//BP86+D3/def2-SVP (smd, solvent = 1,4-Dioxane) level.

Table S1. The calculated NBO 6.0 charge (q) of **IM5** at the BP86+D3/def2-TZVPP (smd, solvent=1,4 Dioxane)//BP86+D3/def2-SVP (smd, solvent = 1,4-Dioxane) level.

	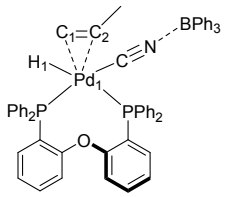 **IM5**
q(Pd_1)	0.355
q(H_1)	-0.085
q(C_1)	-0.505
q(C_2)	-0.252

Table S2. Coordinates and energies (in hatree) of the calculated structures at the bp86+D3/def2-tzvpp(smd,solvent=1,4-Dioxane)//bp86+D3/def2-svp(smd,solvent=1,4-Dioxane) level of theory.

$Pd(PPh_3)_2L$
Free Energy = -4347.872693
Energy = -4348.82199

P	-0.818339	2.057687	-0.844040
P	-1.866630	-1.077679	1.101301
C	-2.341548	2.820095	-0.086448
C	-3.307031	3.590713	-0.773819
C	-2.466878	2.685974	1.311127
C	-4.374881	4.183530	-0.076769
H	-3.224556	3.746121	-1.859969
C	-3.515768	3.298035	2.013815
H	-1.738201	2.064045	1.848258
C	-4.482454	4.043568	1.318377
H	-5.125006	4.769676	-0.632019
H	-3.586915	3.166491	3.105454
H	-5.320017	4.512407	1.859449
C	0.293208	3.563258	-0.879496
C	1.681474	3.348324	-1.010177
C	-0.183840	4.889488	-0.797442
C	2.571773	4.430518	-1.093407
H	2.068996	2.322269	-1.005733
C	0.710570	5.972142	-0.862850
H	-1.258844	5.089673	-0.674804
C	2.089576	5.748301	-1.020096
H	3.652161	4.236565	-1.182885
H	0.322668	7.001402	-0.790592
H	2.788321	6.599039	-1.066443
C	-1.220324	1.959996	-2.658553
C	-0.186589	2.102099	-3.615437
C	-2.517142	1.628676	-3.115233
C	-0.450743	1.935515	-4.984983
H	0.841603	2.333955	-3.297076
C	-2.781891	1.481204	-4.487126
H	-3.329668	1.468442	-2.394203
C	-1.750961	1.633314	-5.430945
H	0.373455	2.042277	-5.707651
H	-3.804265	1.233432	-4.815660
H	-1.956158	1.510092	-6.506300
C	-3.477780	-0.508305	0.387314
C	-4.450710	0.205977	1.116168
C	-3.696166	-0.758462	-0.986606
C	-5.610374	0.678910	0.476188
H	-4.297329	0.409837	2.186412
C	-4.878649	-0.332031	-1.609202
H	-2.931510	-1.288297	-1.574395
C	-5.834841	0.403599	-0.883598
H	-6.345015	1.265365	1.050615
H	-5.035959	-0.556255	-2.676635
H	-6.750567	0.764958	-1.378362
C	-2.163599	-0.884054	2.931960
C	-2.975455	-1.773224	3.670290
C	-1.541290	0.186288	3.607043
C	-3.159402	-1.586485	5.051432
H	-3.465260	-2.619464	3.162649
C	-1.734224	0.383857	4.983252
H	-0.860000	0.843388	3.045984
C	-2.542635	-0.506915	5.710438
H	-3.790453	-2.290719	5.617723
H	-1.223048	1.216691	5.490685
H	-2.684226	-0.367461	6.794335
C	-2.056526	-2.927864	0.925678
C	-3.247741	-3.573759	0.525835
C	-0.922626	-3.723851	1.191189
C	-3.287196	-4.971791	0.378064
H	-4.153317	-2.985716	0.315191
C	-0.959083	-5.119169	1.051966
H	0.016506	-3.236720	1.479581
C	-2.144936	-5.750430	0.634578
H	-4.222637	-5.455009	0.052331
H	-0.048264	-5.707895	1.246282
H	-2.177554	-6.844280	0.506511
Pd	-0.004038	0.023263	0.132021
P	0.799582	-1.408245	-1.599751
C	1.890267	-0.622632	-2.892723
O	3.069952	0.500986	-1.091971
C	3.789784	-0.351232	-0.280520
C	4.839000	-1.141337	-0.777901
C	5.577857	-1.937627	0.110828
C	5.279531	-1.925720	1.484539
C	4.211230	-1.148513	1.963169
C	3.425134	-0.366557	1.089203
C	1.746229	-0.786176	-4.288592
C	2.540022	-0.065245	-5.196220
C	3.502355	0.845861	-4.728232
C	3.688254	1.006234	-3.345179
C	2.904508	0.263678	-2.448831
P	1.824943	0.446035	1.589643
H	5.059592	-1.133813	-1.855781
H	6.392319	-2.569371	-0.276870
H	5.867564	-2.538602	2.185426
H	3.960001	-1.170463	3.034639
H	0.985719	-1.479300	-4.677587
H	2.394827	-0.210949	-6.278263
H	4.114333	1.427027	-5.435731
H	4.437664	1.701153	-2.937829
C	2.355627	2.197425	1.877919
C	1.350926	3.152992	2.147798
C	3.701320	2.615417	1.824799
C	1.682968	4.496982	2.371344
H	0.294671	2.841644	2.156120

C	4.032195	3.966562	2.031064
H	4.496163	1.880878	1.619647
C	3.026625	4.908965	2.306439
H	0.884941	5.230921	2.563610
H	5.086078	4.284271	1.974627
H	3.287172	5.968695	2.456849
C	1.680815	-0.154948	3.348588
C	1.112505	-1.430309	3.559491
C	2.041106	0.617386	4.474021
C	0.914993	-1.934359	4.851956
H	0.780533	-2.012919	2.688953
C	1.824247	0.122587	5.773747
H	2.487728	1.614548	4.338415
C	1.263213	-1.151771	5.967663
H	0.449156	-2.923193	4.986222
H	2.097890	0.742557	6.643060
H	1.085269	-1.529572	6.987072
C	-0.538677	-2.222056	-2.584532
C	-0.969326	-3.530557	-2.263201
C	-1.280749	-1.478757	-3.532425
C	-2.115690	-4.072664	-2.868112
H	-0.420895	-4.128320	-1.520540
C	-2.410930	-2.033933	-4.152914
H	-0.981203	-0.453323	-3.782074
C	-2.840076	-3.331210	-3.818040
H	-2.442003	-5.085714	-2.585203
H	-2.965284	-1.432185	-4.890343
H	-3.737097	-3.760584	-4.292166
C	1.877737	-2.881374	-1.201497
C	2.397410	-3.701858	-2.227673
C	2.196672	-3.177853	0.134341
C	3.210765	-4.802161	-1.913521
H	2.162933	-3.478694	-3.280894
C	3.014291	-4.275139	0.453274
H	1.826260	-2.514102	0.926546
C	3.520415	-5.092555	-0.570809
H	3.608701	-5.436696	-2.721984
H	3.265439	-4.477924	1.506161
H	4.164148	-5.952769	-0.326020

PPh_3

Free Energy **=** -1036.406218

Energy = -1036.625263

P	0.000421	-0.000197	-1.278872
C	-0.538175	1.570350	-0.446783
C	0.120613	2.147169	0.661553
C	-0.358146	3.341347	1.229758
C	-1.502282	3.968221	0.705767
C	-2.165212	3.399813	-0.397443
C	-1.680533	2.215608	-0.975961
H	1.011308	1.658637	1.087308
H	0.166239	3.781876	2.093256
H	-1.876097	4.902598	1.154324
H	-3.060361	3.887215	-0.816421
C	1.629351	-0.319337	-0.446184
C	1.794632	-1.164312	0.673433
C	2.762975	0.333647	-0.984534
C	3.067091	-1.347204	1.243547
H	0.922749	-1.679749	1.106331
C	4.030313	0.160130	-0.404874
H	2.648734	0.988917	-1.864741
C	4.186225	-0.684518	0.709625
H	3.182315	-2.010142	2.116375
H	4.903254	0.680022	-0.831566
H	5.181676	-0.828868	1.159369
C	-1.090369	-1.251438	-0.445904
C	-1.909292	-0.971004	0.670254
C	-1.087304	-2.560879	-0.981483
C	-2.704139	-1.981927	1.239772
H	-1.923499	0.042813	1.100724
C	-1.871234	-3.571901	-0.402210
H	-0.459526	-2.790076	-1.859323
C	-2.685074	-3.283593	0.709032
H	-3.339986	-1.749618	2.109510
H	-1.854237	-4.588683	-0.826735
H	-3.307762	-4.073691	1.158428
H	-2.197757	1.780664	-1.847950

1a

Free Energy **=** -365.0053693

Energy = -365.1163173

C	-2.322449	-0.000123	-0.352550
C	-1.518795	1.255244	-0.157084
C	-0.203147	1.265661	0.128355
C	0.631552	0.000129	0.314981
C	-0.203105	-1.265571	0.129040
C	-1.518752	-1.255367	-0.156406
H	-3.202262	0.000060	0.335143
H	-2.052535	2.216445	-0.255356
H	0.336526	2.218944	0.256448
H	0.336615	-2.218757	0.257650
H	-2.052454	-2.216638	-0.254178
H	-2.783131	-0.000405	-1.370267
C	1.299426	0.000506	1.721330
H	1.933969	-0.898706	1.861238
H	1.933758	0.899939	1.860795
H	0.505255	0.000597	2.494520
C	1.702076	-0.000209	-0.713564
N	2.549060	-0.000442	-1.524372

BPh_3

Free Energy **=** -719.8687141

Energy = -720.0946511

C	1.136610	-1.088034	0.001809
C	2.373765	-0.864000	-0.662194
C	0.970948	-2.335486	0.663807
C	3.386043	-1.836697	-0.677903
H	2.534290	0.090262	-1.190270
C	1.989355	-3.301906	0.675381
H	0.026327	-2.541536	1.193471
C	3.198028	-3.056626	-0.002240
H	4.328987	-1.643358	-1.214736
H	1.840824	-4.253769	1.210801

H	3.995144	-3.817873	-0.003462
C	-1.510900	-0.441262	0.001417
C	-2.506891	0.327145	0.664295
C	-1.937531	-1.623858	-0.662920
C	-3.853695	-0.069507	0.676690
H	-2.210552	1.247452	1.193932
C	-3.286810	-2.011679	-0.678125
H	-1.193143	-2.241733	-1.191491
C	-4.247756	-1.237752	-0.001548
H	-4.602619	0.536126	1.212498
H	-3.592587	-2.924355	-1.215037
H	-5.306013	-1.545886	-0.003009
C	0.372828	1.527457	0.002955
C	-0.438473	2.487799	-0.661306
C	1.536796	2.006624	0.664734
C	-0.099859	3.850304	-0.678330
H	-1.346283	2.151383	-1.188602
C	1.866279	3.371364	0.675817
H	2.187035	1.291292	1.194644
C	1.051257	4.296202	-0.002900
H	-0.737644	4.571036	-1.215453
H	2.765187	3.717664	1.211353
H	1.313845	5.366699	-0.005191
B	-0.000552	-0.000785	0.002783

2a

Free Energy = -117.8994845

Energy = -117.9513885

C	0.129013	-0.453712	0.000025
H	0.158651	-1.560923	-0.000120
C	1.294709	0.219963	0.000133
H	2.264252	-0.305894	-0.000202
H	1.325592	1.324390	-0.000481
C	-1.239632	0.164734	-0.000056
H	-1.199048	1.273914	-0.000146
H	-1.827036	-0.159023	-0.888469
H	-1.826946	-0.158374	0.888803

PhMe

Free Energy = -271.5761436

Energy = -271.6696876

C	-0.923968	0.007955	-0.008034
C	-0.202461	-1.208106	-0.005300
C	1.201857	-1.217684	0.001233
C	1.918008	-0.006412	0.004722
C	1.215153	1.210338	0.001366
C	-0.191408	1.214796	-0.005262
H	-0.754933	-2.162950	-0.008766
H	1.742626	-2.178111	0.001694
H	3.019816	-0.012329	0.008095
H	1.764511	2.165822	0.001960
H	-0.733487	2.175282	-0.009261
C	-2.435365	0.003451	0.005104
H	-2.826210	-0.345491	0.986398
H	-2.854100	1.013675	-0.178177
H	-2.849123	-0.681929	-0.764919

3a

Free Energy = -211.3975666

Energy = -211.4678536

C	1.543070	0.126100	-0.000217
N	2.639840	-0.287003	0.000130
C	0.160794	0.609726	0.000021
C	-0.887010	-0.528683	-0.000053
H	-0.719167	-1.173183	0.889431
H	0.023976	1.262695	0.890577
H	0.024007	1.263001	-0.890321
H	-0.719183	-1.173321	-0.889467
C	-2.317142	0.017292	0.000026
H	-3.059915	-0.806792	-0.000835
H	-2.513598	0.644233	0.896128
H	-2.513274	0.645777	-0.895088

IM1

Free Energy = -3359.896622

Energy = -3360.736515

C	0.425787	2.045069	-3.885383
C	1.128584	0.755901	-3.516478
C	0.461483	-0.461254	-3.341000
C	-1.048594	-0.460930	-3.054108
C	-1.735565	0.813537	-3.532173
C	-1.069511	1.930452	-3.884997
H	0.734213	2.895510	-3.236635
H	2.201856	0.713278	-3.776915
H	0.938296	-1.427135	-3.577280
H	-2.837038	0.790705	-3.524603
H	-1.642189	2.821011	-4.194787
H	0.762857	2.351676	-4.906592
C	-1.757089	-1.710773	-3.603507
H	-2.825853	-1.729799	-3.311284
H	-1.685875	-1.700860	-4.710946
H	-1.280189	-2.641640	-3.235806
C	-1.186286	-0.411869	-1.523832
N	-1.973266	-0.442832	-0.625846
P	1.184800	1.933149	0.148095
C	0.302187	1.986321	1.775365
O	0.760481	-0.380213	2.085048
C	2.119941	-0.554823	2.237768
C	2.852698	0.063691	3.265200
C	4.231628	-0.178695	3.369369
C	4.872966	-1.041094	2.463488
C	4.136040	-1.641625	1.429416
C	2.754190	-1.395814	1.288356
C	-0.273711	3.168285	2.292365
C	-0.952980	3.163739	3.521449
C	-1.101273	1.963207	4.237575
C	-0.533118	0.777714	3.745880
C	0.182061	0.800380	2.539942
P	1.776867	-1.868835	-0.201872
Pd	0.945399	0.080771	-1.278023
H	2.342366	0.742749	3.963735
H	4.807565	0.318079	4.165650

H	5.954104	-1.230848	2.547650
H	4.646619	-2.286798	0.697885
H	-0.207224	4.100166	1.710251
H	-1.393859	4.097048	3.904696
H	-1.667670	1.940532	5.181275
H	-0.642270	-0.176738	4.278636
C	0.723720	-3.271989	0.348082
C	-0.266296	-3.728148	-0.548615
C	0.870215	-3.900188	1.602261
C	-1.098128	-4.801954	-0.199197
H	-0.389066	-3.220572	-1.518362
C	0.029661	-4.971551	1.951685
H	1.638347	-3.545284	2.307534
C	-0.955908	-5.421162	1.055917
H	-1.873209	-5.148332	-0.900480
H	0.141404	-5.454842	2.935392
H	-1.621472	-6.251642	1.338844
C	3.047387	-2.731665	-1.241324
C	3.740789	-1.974697	-2.212923
C	3.355755	-4.101705	-1.090137
C	4.733763	-2.570359	-3.008037
H	3.489536	-0.909008	-2.349452
C	4.343203	-4.698081	-1.893166
H	2.822286	-4.705827	-0.339316
C	5.035905	-3.935065	-2.850457
H	5.267235	-1.967994	-3.760724
H	4.573808	-5.768352	-1.768546
H	5.808680	-4.406275	-3.478627
C	0.640425	3.497113	-0.657996
C	1.543671	4.512292	-1.042567
C	-0.720686	3.596890	-1.033810
C	1.090835	5.612401	-1.793700
H	2.606518	4.443508	-0.762054
C	-1.167012	4.706899	-1.766669
H	-1.434079	2.801604	-0.763820
C	-0.263862	5.714097	-2.154886
H	1.804555	6.396400	-2.094155
H	-2.230894	4.770345	-2.039900
H	-0.616954	6.577640	-2.741046
C	2.936750	2.258258	0.650308
C	3.266860	3.169128	1.678347
C	3.966416	1.550345	-0.002964
C	4.608680	3.369789	2.038492
H	2.469997	3.715113	2.207934
C	5.308494	1.748623	0.362558
H	3.705649	0.820444	-0.787641
C	5.631365	2.659042	1.382715
H	4.857933	4.080021	2.843158
H	6.101947	1.176534	-0.143459
H	6.682730	2.809859	1.675580
B	-3.242953	-0.301910	0.261596
C	-3.609150	1.292820	0.151983
C	-4.194799	1.826911	-1.022399
C	-3.300067	2.208028	1.182801
C	-4.484102	3.196746	-1.153563
H	-4.450445	1.142726	-1.848888
C	-3.582661	3.581558	1.066735
H	-2.820434	1.834953	2.099676
C	-4.184801	4.081738	-0.100452
H	-4.949302	3.576681	-2.078707
H	-3.323318	4.265119	1.891691
H	-4.410884	5.156514	-0.194458
C	-4.375229	-1.290472	-0.411346
C	-5.752181	-0.966490	-0.387943
C	-4.023226	-2.556219	-0.937201
C	-6.728419	-1.855794	-0.875168
H	-6.070439	0.006035	0.023549
C	-4.987371	-3.450628	-1.433426
H	-2.962161	-2.852566	-0.943339
C	-6.350300	-3.101662	-1.407073
H	-7.793969	-1.572669	-0.840951
H	-4.676460	-4.428755	-1.838341
H	-7.112545	-3.798148	-1.793356
C	-3.016802	-0.855988	1.777013
C	-2.004744	-1.785416	2.102346
C	-3.929117	-0.515982	2.806515
C	-1.896928	-2.344355	3.388608
H	-1.272513	-2.073532	1.335977
C	-3.825816	-1.057136	4.099431
H	-4.747458	0.190954	2.588059
C	-2.804542	-1.979468	4.398168
H	-1.085332	-3.057403	3.603088
H	-4.551342	-0.765361	4.877414
H	-2.720778	-2.411446	5.409227

TS1

Free Energy = -3359.885121

Energy = -3360.721487

C	0.713156	2.198919	-3.837829
C	1.440215	0.899417	-3.585726
C	0.768692	-0.309147	-3.432301
C	-0.693855	-0.332713	-3.197124
C	-1.420153	0.913643	-3.527751
C	-0.779753	2.065677	-3.840871
H	1.000449	2.988319	-3.103278
H	2.521969	0.877587	-3.799903
H	1.287400	-1.270666	-3.582547
H	-2.520376	0.872206	-3.490469
H	-1.365582	2.966364	-4.084050
H	1.050331	2.620974	-4.816815
C	-1.405223	-1.625557	-3.531989
H	-2.441523	-1.643459	-3.142361
H	-1.449132	-1.720002	-4.640153
H	-0.860148	-2.507825	-3.143037
C	-1.028114	-0.321317	-1.175332
N	-2.053147	-0.433345	-0.589439
P	1.026821	1.948656	0.187793
C	0.122282	1.851640	1.798633
O	0.914136	-0.431236	2.100423
C	2.289580	-0.454379	2.212866
C	2.979704	0.227156	3.228426
C	4.379410	0.132745	3.290791
C	5.082207	-0.647932	2.356848
C	4.384769	-1.315715	1.336137
C	2.982006	-1.214345	1.235587

C	-0.642168	2.924073	2.309741
C	-1.307057	2.814964	3.541678
C	-1.232880	1.621791	4.279607
C	-0.475149	0.545714	3.793692
C	0.200713	0.665890	2.570946
P	2.010519	-1.793796	-0.220779
Pd	0.947893	0.079801	-1.195963
H	2.418572	0.838168	3.950527
H	4.922200	0.679894	4.077164
H	6.179165	-0.724090	2.411098
H	4.938995	-1.902531	0.587277
H	-0.734093	3.852110	1.725366
H	-1.904037	3.661821	3.914004
H	-1.772645	1.519457	5.233550
H	-0.405788	-0.401703	4.343910
C	1.000480	-3.191463	0.426237
C	-0.070664	-3.652916	-0.368026
C	1.256453	-3.806072	1.670319
C	-0.869035	-4.721576	0.067768
H	-0.294481	-3.147504	-1.320444
C	0.448653	-4.869771	2.108316
H	2.086135	-3.446432	2.299687
C	-0.614147	-5.328076	1.310148
H	-1.711426	-5.066843	-0.551096
H	0.645536	-5.337900	3.086120
H	-1.256208	-6.149790	1.664022
C	3.292992	-2.648269	-1.243343
C	3.994790	-1.867344	-2.190381
C	3.591017	-4.023416	-1.127412
C	4.988747	-2.446168	-2.996100
H	3.750447	-0.795791	-2.290410
C	4.577322	-4.603025	-1.944417
H	3.049860	-4.643991	-0.395682
C	5.279337	-3.817729	-2.876536
H	5.531980	-1.826791	-3.727755
H	4.800451	-5.677993	-1.849997
H	6.051099	-4.276705	-3.514905
C	0.344367	3.469857	-0.596437
C	1.172557	4.553392	-0.967128
C	-1.021045	3.478165	-0.969165
C	0.643157	5.630465	-1.701543
H	2.237690	4.555513	-0.688259
C	-1.543615	4.565781	-1.685361
H	-1.678910	2.632941	-0.707171
C	-0.715270	5.640359	-2.060041
H	1.299672	6.467126	-1.989993
H	-2.608905	4.558435	-1.959160
H	-1.131092	6.484656	-2.632810
C	2.723926	2.460333	0.725333
C	2.921602	3.361682	1.794601
C	3.840805	1.934489	0.045499
C	4.221686	3.729394	2.174444
H	2.053900	3.769435	2.336926
C	5.141724	2.301956	0.429581
H	3.680756	1.215847	-0.775374
C	5.333745	3.198749	1.494139
H	4.368752	4.430203	3.011850
H	6.008382	1.872218	-0.096975
H	6.353695	3.480610	1.800857
B	-3.401209	-0.449218	0.167245
C	-3.893407	1.114979	0.118851
C	-4.412644	1.676238	-1.074809
C	-3.725143	1.991626	1.214392
C	-4.771393	3.033113	-1.165074
H	-4.554171	1.024010	-1.953607
C	-4.066635	3.354671	1.134801
H	-3.305555	1.597346	2.152898
C	-4.599977	3.880953	-0.054141
H	-5.186352	3.433487	-2.105655
H	-3.913037	4.010489	2.008018
H	-4.873790	4.946799	-0.119092
C	-4.396606	-1.496180	-0.614286
C	-5.789829	-1.283568	-0.729987
C	-3.892667	-2.720364	-1.116482
C	-6.636712	-2.235850	-1.329163
H	-6.225296	-0.347352	-0.341700
C	-4.724288	-3.676637	-1.724228
H	-2.815848	-2.929301	-1.008749
C	-6.106682	-3.435721	-1.835945
H	-7.719550	-2.038421	-1.402422
H	-4.296483	-4.618130	-2.109193
H	-6.766509	-4.180921	-2.310021
C	-3.179746	-1.052833	1.669893
C	-2.033826	-1.793208	2.034959
C	-4.204202	-0.935624	2.641670
C	-1.914403	-2.399463	3.299402
H	-1.201933	-1.893916	1.322472
C	-4.088267	-1.517457	3.915905
H	-5.119926	-0.372786	2.391094
C	-2.939589	-2.260625	4.250508
H	-1.003118	-2.970406	3.539448
H	-4.902969	-1.400844	4.650618
H	-2.848377	-2.728512	5.244945

IM2

Free Energy **=** -3359.921676

Energy = -3360.759954

C	3.451067	1.080901	-2.870821
C	2.789455	-0.250888	-2.554222
C	1.592370	-0.637421	-3.256956
C	0.704163	0.419278	-3.621255
C	1.251357	1.771406	-3.806704
C	2.543467	2.080728	-3.521780
H	3.899407	1.526417	-1.951941
H	3.483579	-1.060244	-2.275200
H	1.345627	-1.693097	-3.457735
H	0.572904	2.537799	-4.214154
H	2.930087	3.094630	-3.711087
H	4.333284	0.897549	-3.536467
C	-0.671418	0.134136	-4.169284
H	-1.407964	0.872510	-3.791858
H	-0.668368	0.214925	-5.279761
H	-1.025229	-0.877690	-3.892018
C	-0.931668	0.031241	-0.776922
N	-2.054810	0.090502	-0.435029

P	1.579258	1.759989	0.190715
C	0.375264	2.111014	1.554535
O	0.200302	-0.272917	1.961232
C	1.356543	-0.802830	2.480515
C	1.934620	-0.340093	3.674884
C	3.075786	-0.981746	4.179653
C	3.620542	-2.093052	3.512160
C	3.053235	-2.530128	2.303900
C	1.938516	-1.868541	1.744189
C	-0.062667	3.414084	1.882856
C	-1.040686	3.620161	2.869950
C	-1.602555	2.523432	3.544078
C	-1.169297	1.221604	3.249877
C	-0.181472	1.027071	2.275411
P	1.305999	-2.133766	0.033103
Pd	1.004584	-0.087062	-1.265544
H	1.486309	0.517817	4.196807
H	3.534261	-0.613381	5.110670
H	4.497776	-2.614532	3.925183
H	3.497482	-3.387625	1.776295
H	0.347716	4.278408	1.339440
H	-1.378990	4.643434	3.094760
H	-2.394741	2.670388	4.293817
H	-1.602142	0.345034	3.751209
C	-0.232282	-3.129880	0.231262
C	-1.200202	-3.112726	-0.797607
C	-0.461835	-3.904575	1.389353
C	-2.386890	-3.852000	-0.668372
H	-1.044227	-2.489063	-1.691059
C	-1.649454	-4.645719	1.513637
H	0.282192	-3.913300	2.201637
C	-2.613840	-4.615599	0.489761
H	-3.152253	-3.797432	-1.458017
H	-1.830762	-5.235626	2.426161
H	-3.558982	-5.169122	0.603249
C	2.494073	-3.320324	-0.730946
C	3.875770	-3.005175	-0.778261
C	2.039642	-4.472837	-1.411802
C	4.775717	-3.829009	-1.472430
H	4.255833	-2.114741	-0.253453
C	2.943226	-5.287865	-2.116046
H	0.972067	-4.741697	-1.389043
C	4.312113	-4.972067	-2.148994
H	5.847201	-3.572802	-1.487317
H	2.569879	-6.183362	-2.638217
H	5.017538	-5.615208	-2.698539
C	1.630931	3.374096	-0.688899
C	2.806027	4.136300	-0.839158
C	0.442188	3.789153	-1.336589
C	2.792377	5.303962	-1.626468
H	3.738312	3.819730	-0.345359
C	0.428657	4.963939	-2.099811
H	-0.475477	3.183663	-1.246428
C	1.606887	5.722210	-2.253150
H	3.717400	5.890836	-1.744821
H	-0.506095	5.282596	-2.587875
H	1.598167	6.639159	-2.863799
C	3.174416	1.652870	1.117610
C	3.478686	2.539367	2.174881
C	4.069802	0.609641	0.809016
C	4.663225	2.376603	2.910629
H	2.777455	3.348808	2.433471
C	5.252533	0.445509	1.549049
H	3.811298	-0.092302	0.001124
C	5.549262	1.327380	2.602147
H	4.891513	3.066536	3.738732
H	5.935802	-0.385501	1.312984
H	6.470323	1.192838	3.191331
B	-3.554038	0.166291	-0.038839
C	-4.017030	1.706079	-0.339778
C	-5.264774	2.041896	-0.910810
C	-3.167530	2.779754	0.025711
C	-5.647437	3.383080	-1.113288
H	-5.953452	1.232414	-1.208284
C	-3.532427	4.121354	-0.175794
H	-2.193544	2.554802	0.489381
C	-4.780888	4.429772	-0.750245
H	-6.628618	3.612856	-1.562265
H	-2.840472	4.928628	0.119644
H	-5.077150	5.479512	-0.912195
C	-4.320411	-0.948784	-0.969933
C	-5.277734	-1.849446	-0.449661
C	-4.027837	-1.057266	-2.351807
C	-5.900080	-2.821309	-1.257181
H	-5.529261	-1.801872	0.622855
C	-4.633905	-2.026664	-3.169737
H	-3.291131	-0.367199	-2.796535
C	-5.574143	-2.921063	-2.621498
H	-6.637910	-3.512112	-0.815390
H	-4.373847	-2.087625	-4.240175
H	-6.050989	-3.686879	-3.255273
C	-3.662591	-0.210793	1.551288
C	-2.999533	-1.356690	2.052634
C	-4.446590	0.526831	2.466445
C	-3.110216	-1.754939	3.394761
H	-2.371226	-1.945968	1.371217
C	-4.565205	0.142957	3.817047
H	-4.973002	1.430484	2.115757
C	-3.896285	-1.001437	4.288982
H	-2.572679	-2.652338	3.744169
H	-5.184619	0.741578	4.506278
H	-3.986763	-1.304400	5.345316

IM2'

Free Energy = -3359.890975

Energy = -3360.727092

B	-3.887720	0.584451	-0.386049
C	-4.436141	-0.254128	-1.683851
C	-3.704907	-1.323424	-2.255873
C	-5.715194	0.010328	-2.229455
C	-4.222109	-2.095326	-3.311791
H	-2.705291	-1.572147	-1.860216
C	-6.245452	-0.756627	-3.283714
H	-6.310273	0.843288	-1.817332
C	-5.499271	-1.816093	-3.831450

H	-3.624505	-2.925530	-3.724674
H	-7.246140	-0.522322	-3.684540
H	-5.909738	-2.417569	-4.659455
C	-4.315969	-0.136455	1.023686
C	-5.407970	-1.027760	1.129205
C	-3.586204	0.123156	2.209189
C	-5.744089	-1.645913	2.349888
H	-5.998388	-1.261138	0.227253
C	-3.892984	-0.504507	3.427931
H	-2.737139	0.824361	2.168950
C	-4.978226	-1.397921	3.503054
H	-6.600263	-2.340008	2.396489
H	-3.276639	-0.302665	4.319667
H	-5.225583	-1.896048	4.454997
C	-4.328756	2.163156	-0.427184
C	-3.636104	3.100346	-1.232235
C	-5.437296	2.647533	0.306273
C	-4.021096	4.451342	-1.300953
H	-2.765372	2.763822	-1.821581
C	-5.838935	3.995492	0.241201
H	-5.996312	1.950055	0.953174
C	-5.128699	4.906508	-0.560848
H	-3.453621	5.153726	-1.934524
H	-6.708353	4.338992	0.826842
H	-5.435845	5.964277	-0.609988
C	3.866070	-3.185200	-2.503848
C	4.351769	-1.788712	-2.254553
C	3.547385	-0.697155	-2.346844
C	2.115790	-0.787180	-2.644642
C	1.622954	-2.144171	-2.946354
C	2.414382	-3.247462	-2.875095
H	4.484460	-3.669092	-3.301187
H	5.418955	-1.652694	-2.012078
H	3.974916	0.303582	-2.200523
H	0.568864	-2.240911	-3.258286
H	1.994932	-4.237528	-3.123167
H	4.063054	-3.827402	-1.609561
C	1.463497	0.349910	-3.397297
H	0.558987	0.828924	-2.856336
H	2.161777	1.187523	-3.584536
H	1.006387	0.013460	-4.350934
C	-1.174774	0.480860	-0.591866
N	-2.342682	0.545954	-0.455707
P	0.554755	-1.800006	0.365379
C	2.097375	-2.784598	0.585546
O	3.314100	-0.685880	0.712741
C	3.079337	0.075926	1.841490
C	3.273124	-0.419486	3.141780
C	3.051170	0.426744	4.238529
C	2.652544	1.759475	4.037718
C	2.439047	2.236283	2.734794
C	2.633485	1.402544	1.612689
C	2.146232	-4.196758	0.602129
C	3.362188	-4.872995	0.790738
C	4.556417	-4.147356	0.957030
C	4.530810	-2.742959	0.948003
C	3.311749	-2.071749	0.768539
P	2.130912	1.882622	-0.104130
Pd	0.719276	0.009024	-1.081694
H	3.574242	-1.466952	3.287831
H	3.185101	0.033848	5.258338
H	2.479697	2.423731	4.898247
H	2.082503	3.266907	2.586556
H	1.216781	-4.773569	0.482175
H	3.376229	-5.973859	0.807549
H	5.512443	-4.675293	1.097926
H	5.446835	-2.147189	1.073406
C	3.719251	2.371756	-0.902290
C	3.654393	3.061564	-2.137278
C	4.978425	1.971408	-0.405229
C	4.823928	3.330364	-2.864373
H	2.678432	3.396880	-2.526082
C	6.146474	2.233960	-1.142709
H	5.049632	1.445295	0.558693
C	6.074177	2.906492	-2.374838
H	4.759054	3.871908	-3.821675
H	7.123012	1.912314	-0.746228
H	6.991111	3.108174	-2.950861
C	1.310171	3.520847	0.164739
C	-0.099828	3.578465	0.219036
C	2.055572	4.710441	0.344737
C	-0.755654	4.798771	0.457609
H	-0.697111	2.667789	0.060969
C	1.397297	5.929413	0.575894
H	3.156038	4.680521	0.306729
C	-0.008351	5.975739	0.634815
H	-1.856717	4.820861	0.484807
H	1.987133	6.850161	0.712811
H	-0.522397	6.933777	0.813670
C	-0.814440	-2.970869	-0.008410
C	-2.051331	-2.816770	0.660029
C	-0.717002	-3.899633	-1.072742
C	-3.161323	-3.587748	0.277327
H	-2.170766	-2.077337	1.465540
C	-1.830609	-4.669132	-1.444453
H	0.232299	-4.019801	-1.610868
C	-3.056251	-4.515432	-0.771265
H	-4.117930	-3.433489	0.797700
H	-1.739618	-5.390738	-2.272166
H	-3.933752	-5.107034	-1.075364
C	0.198113	-1.322172	2.121349
C	0.247932	-2.326676	3.115222
C	-0.123465	-0.002143	2.488245
C	-0.020996	-2.009497	4.454626
H	0.495671	-3.364073	2.839550
C	-0.380530	0.313728	3.832790
H	-0.165808	0.788457	1.728008
C	-0.333749	-0.686191	4.816650
H	0.013766	-2.800555	5.220496
H	-0.621604	1.352322	4.105803
H	-0.540398	-0.435396	5.869222

IM3

Free Energy **=** -3359.913389

Energy = -3360.749703

B	3.703862	-0.602519	0.433732	C	-3.525003	-0.546850	2.753374
C	4.492739	-0.512120	-1.005330	C	-3.473730	-0.199120	1.386280
C	4.305503	0.637809	-1.810889	C	-1.703073	4.401668	-1.113559
C	5.266008	-1.559040	-1.552466	C	-2.694781	5.267277	-1.604522
C	4.860020	0.746987	-3.095841	C	-4.032803	4.842028	-1.674603
H	3.688825	1.460871	-1.420368	C	-4.380368	3.555872	-1.230964
C	5.824128	-1.467554	-2.844395	C	-3.385308	2.705564	-0.725651
H	5.427260	-2.476107	-0.960242	P	-2.750690	-1.303527	0.092174
C	5.623111	-0.313893	-3.623129	Pd	-0.829268	-0.397647	-0.899233
H	4.688410	1.659182	-3.692374	H	-4.255349	3.148114	1.691979
H	6.418089	-2.305492	-3.246838	H	-4.303955	2.504665	4.119247
H	6.057539	-0.241793	-4.633989	H	-3.848107	0.123653	4.792741
C	3.953539	0.687849	1.412691	H	-3.280830	-1.573550	3.063066
C	5.063609	1.553987	1.298201	H	-0.655526	4.738193	-1.085330
C	3.011040	0.987746	2.426263	H	-2.415822	6.278090	-1.940663
C	5.217010	2.675666	2.137558	H	-4.810943	5.513487	-2.070297
H	5.817692	1.358099	0.517166	H	-5.418800	3.193373	-1.261726
C	3.139427	2.109990	3.260421	C	-4.166695	-1.955781	-0.899644
H	2.134405	0.331186	2.550489	C	-4.053192	-3.227253	-1.514608
C	4.248324	2.966572	3.115164	C	-5.317927	-1.176568	-1.153140
H	6.093580	3.334821	2.018029	C	-5.065510	-3.701583	-2.365263
H	2.362972	2.323858	4.014103	H	-3.182333	-3.868193	-1.305652
H	4.357596	3.853104	3.761571	C	-6.328454	-1.658577	-2.001626
C	3.974468	-2.013740	1.208508	H	-5.427964	-0.185483	-0.691649
C	3.092185	-3.118192	1.145511	C	-6.205640	-2.918306	-2.614247
C	5.174479	-2.196376	1.938148	H	-4.962251	-4.694809	-2.830774
C	3.387547	-4.344580	1.772289	H	-7.223119	-1.041542	-2.182977
H	2.146886	-3.019627	0.585183	H	-7.000066	-3.291358	-3.279951
C	5.483670	-3.415352	2.566859	C	-2.234201	-2.777251	1.095189
H	5.883161	-1.353688	2.015600	C	-0.878024	-2.907293	1.467019
C	4.588322	-4.498785	2.487754	C	-3.170303	-3.728456	1.563646
H	2.679423	-5.187416	1.695188	C	-0.462259	-3.963706	2.295496
H	6.427806	-3.522449	3.127107	H	-0.140886	-2.173832	1.101754
H	4.826043	-5.456116	2.980214	C	-2.750380	-4.789334	2.383370
C	0.353665	-3.099346	-2.057809	H	-4.234020	-3.636162	1.293337
C	-0.745856	-2.074178	-2.275325	C	-1.397237	-4.908343	2.752118
C	-0.532283	-1.094193	-3.333673	H	0.599620	-4.041522	2.577461
C	0.741512	-0.818955	-3.824481	H	-3.487973	-5.525196	2.741835
C	1.879651	-1.545743	-3.285254	H	-1.072314	-5.739897	3.397738
C	1.717493	-2.586713	-2.417600	C	0.799471	2.688638	-0.741956
H	0.330689	-3.505819	-1.023960	C	1.780352	3.242714	0.103252
H	-1.403859	-0.564876	-3.757686	C	0.977589	2.734818	-2.144560
H	2.895570	-1.216479	-3.558406	C	2.911899	3.869136	-0.452097
H	2.604040	-3.093704	-2.003269	H	1.683826	3.177448	1.196353
H	0.141417	-3.988001	-2.711545	C	2.094716	3.381314	-2.692610
C	1.001064	0.246672	-4.850981	H	0.228665	2.269305	-2.806299
H	1.470356	-0.181586	-5.764485	C	3.062910	3.955705	-1.845693
H	0.077870	0.780791	-5.153085	H	3.682953	4.272493	0.221474
H	1.729545	0.988439	-4.454665	H	2.218627	3.426139	-3.786199
C	1.143901	-0.537731	-0.471006	H	3.951323	4.444468	-2.275523
N	2.216251	-0.548728	0.014761	C	-0.677718	2.094048	1.709002
P	-0.737205	1.874997	-0.121290	C	-0.805091	3.367816	2.306477
C	-2.025616	3.098703	-0.669014	C	-0.480067	0.960159	2.522202
O	-3.756132	1.431753	-0.321627	C	-0.724133	3.501319	3.700944
C	-3.766584	1.138078	1.032017	H	-0.969056	4.257642	1.678068
C	-4.064316	2.109898	2.001115	C	-0.404657	1.097153	3.918142
C	-4.090052	1.741836	3.354783	H	-0.389360	-0.033429	2.058483
C	-3.834170	0.412429	3.730757	C	-0.522967	2.366059	4.508835

H	-0.820001	4.497565	4.161306
H	-0.249888	0.203924	4.542845
H	-0.461293	2.472597	5.603550
H	-1.755435	-2.517568	-2.274129

TS2

Free Energy = -3359.901864

Energy = -3360.731102

B	3.891563	0.421441	0.085963
C	4.691784	0.218394	1.498416
C	4.206788	-0.690372	2.472276
C	5.920483	0.859855	1.773245
C	4.909179	-0.946009	3.662435
H	3.255878	-1.220431	2.285308
C	6.635816	0.610745	2.960938
H	6.327359	1.574168	1.037115
C	6.131647	-0.293172	3.912545
H	4.504441	-1.661279	4.398756
H	7.592021	1.128845	3.146169
H	6.687788	-0.488427	4.844508
C	4.094800	-0.872190	-0.904037
C	5.120050	-1.827351	-0.717131
C	3.228704	-1.074493	-2.006370
C	5.263097	-2.938838	-1.570986
H	5.815913	-1.704972	0.129515
C	3.347418	-2.186012	-2.857847
H	2.424495	-0.343197	-2.192593
C	4.368851	-3.129598	-2.639238
H	6.071402	-3.667931	-1.392400
H	2.632006	-2.325645	-3.684640
H	4.467136	-4.007121	-3.299279
C	4.229698	1.843080	-0.659399
C	4.938546	1.921033	-1.880478
C	3.811369	3.068436	-0.083081
C	5.217124	3.156362	-2.499895
H	5.276880	0.988898	-2.363589
C	4.080354	4.306963	-0.689380
H	3.246384	3.045518	0.864898
C	4.787027	4.356277	-1.906349
H	5.771427	3.180805	-3.453316
H	3.730500	5.240250	-0.217394
H	4.998452	5.324616	-2.389346
C	-1.106423	-0.612731	3.331346
C	-2.320765	-0.053681	2.745563
C	-2.759075	1.230377	3.161709
C	-2.076285	1.958706	4.148398
C	-0.924207	1.374765	4.761522
C	-0.463910	0.121428	4.398470
H	-1.006132	-1.713667	3.346265
H	-3.014869	-0.710880	2.201610
H	-3.683826	1.639438	2.726724
H	-0.408437	1.930959	5.561753
H	0.416966	-0.321300	4.888617
H	-0.125866	-0.572700	2.295320
C	-2.552923	3.311949	4.609508
H	-3.554684	3.555767	4.207588
H	-2.596473	3.363048	5.718770
H	-1.852928	4.112134	4.283004
C	1.224450	0.513688	0.660095
N	2.380375	0.472103	0.436617
P	-1.110270	-2.105821	0.030481
C	-2.773397	-2.868027	0.274552
O	-3.730300	-0.695906	-0.274956
C	-3.476198	-0.442901	-1.615444
C	-3.943763	-1.301047	-2.625428
C	-3.698681	-0.984136	-3.969556
C	-3.008879	0.192980	-4.303805
C	-2.530030	1.033465	-3.287517
C	-2.735475	0.724223	-1.924832
C	-3.009540	-4.200988	0.682934
C	-4.307767	-4.651695	0.975957
C	-5.401471	-3.773862	0.871293
C	-5.198324	-2.451478	0.443117
C	-3.901384	-2.014974	0.134308
P	-1.839343	1.623363	-0.576737
Pd	-0.713325	0.165515	0.943409
H	-4.484420	-2.218959	-2.352347
H	-4.050384	-1.667011	-4.758405
H	-2.816675	0.445448	-5.357704
H	-1.947456	1.927734	-3.554936
H	-2.160409	-4.895755	0.774698
H	-4.464375	-5.695843	1.289050
H	-6.418785	-4.120323	1.111511
H	-6.033932	-1.744667	0.329524
C	-3.093008	2.718804	0.202443
C	-2.628165	3.782731	1.010066
C	-4.479974	2.494465	0.079582
C	-3.542328	4.630543	1.653264
H	-1.545204	3.952490	1.122908
C	-5.390141	3.327476	0.754518
H	-4.855145	1.670268	-0.545093
C	-4.925634	4.400404	1.535303
H	-3.171798	5.470389	2.261378
H	-6.472008	3.143714	0.655469
H	-5.641755	5.060011	2.050663
C	-0.781471	2.804878	-1.530287
C	0.542097	2.431892	-1.847863
C	-1.275118	4.046946	-1.992500
C	1.367743	3.282135	-2.600440
H	0.950350	1.480315	-1.482276
C	-0.446120	4.898902	-2.742340
H	-2.309322	4.351080	-1.768048
C	0.875237	4.520811	-3.044672
H	2.406066	2.981495	-2.810676
H	-0.837139	5.868638	-3.090312
H	1.528057	5.197195	-3.619026
C	0.126526	-3.200187	0.840858
C	1.433819	-3.202600	0.297668
C	-0.086985	-3.781980	2.114406
C	2.500803	-3.768216	1.012994
H	1.637423	-2.735967	-0.678510
C	0.985144	-4.354598	2.821298
H	-1.092044	-3.789747	2.565591
C	2.282071	-4.343749	2.277622
H	3.509719	-3.733817	0.574344

H	0.802508	-4.808210	3.809002
H	3.123357	-4.778079	2.840301
C	-0.800924	-2.352717	-1.773998
C	-1.140575	-3.560080	-2.423542
C	-0.219526	-1.306528	-2.514372
C	-0.904871	-3.707394	-3.799046
H	-1.597554	-4.384864	-1.854041
C	0.010150	-1.453364	-3.892398
H	0.044899	-0.368844	-2.007052
C	-0.332570	-2.653202	-4.536619
H	-1.171652	-4.651101	-4.301256
H	0.456684	-0.621449	-4.458787
H	-0.154940	-2.769816	-5.617599

IM4

Free Energy = -3359.927016

Energy = -3360.760172

B	-3.787544	0.785621	-0.060947
C	-4.506696	0.350840	-1.470851
C	-4.307404	-0.955951	-1.981032
C	-5.330133	1.213012	-2.228964
C	-4.886139	-1.383663	-3.186949
H	-3.680570	-1.660261	-1.410488
C	-5.920811	0.797557	-3.439123
H	-5.515948	2.237544	-1.864786
C	-5.698398	-0.502361	-3.926263
H	-4.699173	-2.407479	-3.552861
H	-6.559429	1.495732	-4.006271
H	-6.157089	-0.828524	-4.874463
C	-4.123398	-0.254608	1.163959
C	-5.222331	-1.143957	1.144903
C	-3.291388	-0.297141	2.309201
C	-5.460164	-2.053247	2.194630
H	-5.902355	-1.138710	0.276984
C	-3.504047	-1.208966	3.356661
H	-2.434167	0.392489	2.370910
C	-4.591616	-2.101116	3.299413
H	-6.324230	-2.737158	2.143165
H	-2.810610	-1.231556	4.213049
H	-4.763287	-2.823999	4.113944
C	-4.076579	2.345321	0.340032
C	-3.420147	3.407604	-0.329502
C	-5.035909	2.701811	1.316166
C	-3.704868	4.756016	-0.046153
H	-2.667738	3.171085	-1.101912
C	-5.328176	4.046534	1.613214
H	-5.566258	1.902447	1.861319
C	-4.662162	5.081963	0.933099
H	-3.179284	5.557034	-0.592924
H	-6.080963	4.288872	2.382205
H	-4.889629	6.136341	1.161582
C	2.823366	-0.085243	-3.878674
C	1.801227	0.833643	-3.577759
C	0.463966	0.402862	-3.458216
C	0.114596	-0.956549	-3.674506
C	1.151696	-1.860288	-3.996278
C	2.489540	-1.434007	-4.090358
H	3.867678	0.258385	-3.942686
H	2.043196	1.896936	-3.439837
H	-0.334743	1.142088	-3.281518
H	0.901041	-2.916102	-4.190272
H	3.277807	-2.164043	-4.335940
H	2.310339	-0.424385	-1.043417
C	-1.322813	-1.389735	-3.550500
H	-1.511037	-2.368705	-4.032864
H	-1.608759	-1.489839	-2.483471
H	-2.016710	-0.643405	-3.986747
C	-1.090747	0.558415	-0.463174
N	-2.252777	0.661786	-0.306326
P	0.684920	-1.974314	0.318673
C	2.218559	-3.014794	0.398453
O	3.650936	-1.033450	0.591356
C	3.378578	-0.331113	1.753157
C	3.550819	-0.938901	3.008999
C	3.344987	-0.195668	4.178704
C	2.975675	1.156193	4.091602
C	2.775078	1.746695	2.835095
C	2.956813	1.022159	1.633331
C	2.170589	-4.426168	0.322194
C	3.339871	-5.203105	0.348577
C	4.595933	-4.582077	0.448934
C	4.672068	-3.184483	0.545491
C	3.498811	-2.412799	0.537108
P	2.343760	1.723495	0.018272
Pd	0.866732	0.073822	-0.762716
H	3.842666	-1.998309	3.056883
H	3.470316	-0.680555	5.159056
H	2.812295	1.749814	5.003925
H	2.431789	2.790182	2.789395
H	1.195752	-4.929310	0.233474
H	3.264981	-6.299938	0.287420
H	5.518535	-5.183236	0.460896
H	5.637146	-2.664278	0.638994
C	3.813943	2.131397	-1.014923
C	3.711093	3.178868	-1.960512
C	4.981533	1.338459	-0.993184
C	4.755066	3.423364	-2.866974
H	2.808093	3.809262	-1.990812
C	6.023152	1.588372	-1.902967
H	5.075126	0.510542	-0.277401
C	5.913785	2.626280	-2.844626
H	4.659701	4.242257	-3.597650
H	6.929340	0.962324	-1.873546
H	6.731095	2.817126	-3.558013
C	1.681616	3.373074	0.518466
C	0.288160	3.533260	0.670385
C	2.543219	4.457446	0.812121
C	-0.239601	4.756082	1.121135
H	-0.395098	2.703146	0.431135
C	2.010506	5.679923	1.250995
H	3.633368	4.343001	0.703395
C	0.619565	5.829698	1.409667
H	-1.330292	4.861557	1.231586
H	2.687090	6.520092	1.475410
H	0.204970	6.789558	1.757024

C	-0.654058	-3.097187	-0.241170
C	-1.909003	-3.075245	0.407465
C	-0.495628	-3.841517	-1.433841
C	-2.985279	-3.804901	-0.126722
H	-2.064348	-2.477952	1.318779
C	-1.571643	-4.577685	-1.951448
H	0.467716	-3.826524	-1.966802
C	-2.820003	-4.559191	-1.301020
H	-3.960589	-3.759199	0.381280
H	-1.439102	-5.155697	-2.879952
H	-3.668654	-5.124224	-1.717739
C	0.340019	-1.712612	2.121371
C	0.337866	-2.822995	2.995231
C	0.123540	-0.421557	2.638651
C	0.129435	-2.636750	4.369982
H	0.502776	-3.837998	2.600187
C	-0.077910	-0.238070	4.016504
H	0.126234	0.445099	1.962981
C	-0.073320	-1.341928	4.883968
H	0.126398	-3.507404	5.044885
H	-0.239542	0.777690	4.408084
H	-0.231819	-1.195960	5.964293

IM5

Free Energy **=** -3206.268279

Energy = -3207.059956

B	3.466526	-0.331291	0.067733
C	3.580040	-1.385459	-1.175289
C	2.466371	-1.825436	-1.926244
C	4.854505	-1.841099	-1.595208
C	2.615504	-2.644069	-3.061264
H	1.450797	-1.536288	-1.615117
C	5.016318	-2.664246	-2.723390
H	5.746752	-1.540878	-1.019760
C	3.892629	-3.063673	-3.471472
H	1.721746	-2.962571	-3.622584
H	6.024834	-2.996978	-3.021797
H	4.013191	-3.704894	-4.360389
C	3.870891	1.200829	-0.372485
C	4.471973	1.530842	-1.607231
C	3.641106	2.269621	0.528702
C	4.831195	2.854824	-1.927247
H	4.659931	0.731624	-2.343015
C	3.965597	3.599755	0.212891
H	3.206863	2.042533	1.518386
C	4.570369	3.898361	-1.022889
H	5.303926	3.074465	-2.899511
H	3.757353	4.407295	0.934733
H	4.838613	4.937507	-1.275574
C	4.348571	-0.843454	1.352469
C	3.848459	-1.811583	2.256619
C	5.669628	-0.386734	1.572252
C	4.619893	-2.302138	3.324799
H	2.821525	-2.191052	2.117902
C	6.457032	-0.875667	2.632131
H	6.089495	0.381367	0.900466
C	5.934143	-1.835891	3.516105
H	4.196383	-3.053601	4.012737
H	7.484066	-0.498678	2.773422
H	6.544945	-2.217121	4.351067
C	0.876510	-0.180787	0.897571
N	1.989431	-0.261507	0.532234
P	-1.268331	1.959235	0.035761
C	-0.107458	1.988343	-1.400391
O	-0.645110	-0.338607	-1.882409
C	-1.983146	-0.494386	-2.169684
C	-2.608921	0.140841	-3.254332
C	-3.970052	-0.104400	-3.496644
C	-4.693784	-0.986100	-2.674465
C	-4.062598	-1.605155	-1.582466
C	-2.703153	-1.355636	-1.303700
C	0.691064	3.111674	-1.710260
C	1.592090	3.080704	-2.785356
C	1.717930	1.921419	-3.567153
C	0.936535	0.792639	-3.278406
C	0.033398	0.831964	-2.206952
P	-1.858423	-1.873429	0.247302
Pd	-1.067309	0.048963	1.435830
H	-2.031030	0.829821	-3.888070
H	-4.467979	0.403480	-4.337112
H	-5.759251	-1.179439	-2.872521
H	-4.637441	-2.271367	-0.920423
H	0.621344	4.017465	-1.089680
H	2.220406	3.959269	-2.991033
H	2.444824	1.883716	-4.392646
H	1.032882	-0.137695	-3.854888
C	-0.596108	-3.105265	-0.268567
C	-0.668280	-3.780993	-1.505776
C	0.459358	-3.391622	0.623341
C	0.303814	-4.740194	-1.836155
H	-1.484201	-3.554385	-2.210817
C	1.434718	-4.341135	0.282214
H	0.525676	-2.850555	1.580111
C	1.357105	-5.017197	-0.947394
H	0.248966	-5.261005	-2.805215
H	2.274181	-4.532966	0.968086
H	2.136066	-5.743624	-1.225751
C	-3.142530	-2.888489	1.104632
C	-4.027702	-2.257847	2.006665
C	-3.274129	-4.274672	0.865006
C	-5.038619	-2.995527	2.644434
H	-3.913962	-1.181027	2.214574
C	-4.280241	-5.011330	1.513074
H	-2.586066	-4.782933	0.171602
C	-5.166007	-4.374678	2.400259
H	-5.723410	-2.491542	3.345026
H	-4.370385	-6.092660	1.322216
H	-5.952322	-4.955602	2.908139
C	-0.849946	3.476686	0.984395
C	-1.786367	4.497417	1.247152
C	0.428818	3.527580	1.585918
C	-1.443478	5.556884	2.108092
H	-2.786887	4.464401	0.788652
C	0.767627	4.591123	2.433287
H	1.156555	2.727574	1.382261

C	-0.171108	5.606381	2.702242
H	-2.180793	6.348990	2.314723
H	1.767532	4.621469	2.894429
H	0.091082	6.436127	3.377664
C	-2.899446	2.325957	-0.742041
C	-2.990414	3.275920	-1.785133
C	-4.058640	1.654368	-0.309086
C	-4.230884	3.547946	-2.381642
H	-2.084995	3.796060	-2.136124
C	-5.298164	1.925852	-0.912844
H	-3.979969	0.900597	0.490086
C	-5.386514	2.871896	-1.947720
H	-4.294808	4.288425	-3.194847
H	-6.196015	1.381781	-0.580520
H	-6.357638	3.078205	-2.425280
H	-2.577707	0.283708	1.801790
C	-0.575205	0.809510	3.522401
C	-0.749920	-0.586073	3.556948
H	-1.678527	-1.021882	3.965057
H	0.125775	-1.255220	3.543526
H	0.457114	1.192916	3.422267
C	-1.574941	1.796768	4.072744
H	-1.279335	2.092213	5.105359
H	-1.615776	2.730452	3.475107
H	-2.597213	1.367957	4.119386

TS3

Free Energy **=** -3206.252007

Energy = -3207.041773

B	3.485321	-0.198587	0.093438
C	3.614111	-1.235953	-1.165117
C	2.518763	-1.561242	-1.997890
C	4.871003	-1.782181	-1.522276
C	2.668967	-2.359484	-3.145665
H	1.514661	-1.199960	-1.733147
C	5.033749	-2.589670	-2.663123
H	5.748290	-1.569936	-0.887698
C	3.930804	-2.877283	-3.488134
H	1.787981	-2.590444	-3.766930
H	6.028644	-2.997307	-2.910389
H	4.053555	-3.507049	-4.384917
C	3.850176	1.345092	-0.335313
C	4.581089	1.675433	-1.498425
C	3.484264	2.418268	0.513096
C	4.937620	3.005022	-1.797816
H	4.880838	0.869862	-2.189513
C	3.815965	3.751425	0.219937
H	2.933424	2.193382	1.443003
C	4.553104	4.051154	-0.941548
H	5.513863	3.225441	-2.712383
H	3.501499	4.560860	0.900247
H	4.823586	5.093827	-1.176956
C	4.401890	-0.695690	1.360403
C	3.948131	-1.687818	2.263102
C	5.713400	-0.203429	1.559906
C	4.754436	-2.166527	3.310985
H	2.929515	-2.095954	2.142612
C	6.535213	-0.679591	2.599240
H	6.098132	0.580714	0.885750
C	6.057818	-1.663711	3.482741
H	4.366573	-2.937459	3.998518
H	7.553423	-0.274043	2.724769
H	6.695467	-2.035251	4.301912
C	0.902543	-0.176240	0.957685
N	2.013114	-0.182805	0.573459
P	-1.418466	2.001847	0.195174
C	-0.207498	2.275899	-1.176005
O	-0.500549	-0.043087	-1.843985
C	-1.790191	-0.291357	-2.249011
C	-2.399042	0.390164	-3.315523
C	-3.703013	0.038129	-3.696808
C	-4.386215	-0.995787	-3.031874
C	-3.776440	-1.657293	-1.952972
C	-2.480075	-1.299273	-1.528814
C	0.494177	3.487364	-1.363131
C	1.469269	3.610614	-2.365296
C	1.766727	2.520495	-3.198239
C	1.074862	1.309365	-3.041718
C	0.098118	1.198225	-2.043238
P	-1.688666	-1.898090	0.024329
Pd	-1.029620	-0.133927	1.456360
H	-1.849711	1.194149	-3.827222
H	-4.187176	0.579239	-4.524540
H	-5.403890	-1.278034	-3.342489
H	-4.323405	-2.448008	-1.416928
H	0.291553	4.340906	-0.698815
H	2.020759	4.555749	-2.474763
H	2.552741	2.603401	-3.963491
H	1.299283	0.434255	-3.667047
C	-0.379801	-3.073235	-0.509633
C	-0.458439	-3.748377	-1.747178
C	0.700000	-3.333134	0.360177
C	0.536644	-4.673573	-2.102301
H	-1.295655	-3.545728	-2.434150
C	1.699303	-4.248469	-0.006412
H	0.766853	-2.798568	1.320242
C	1.617789	-4.920216	-1.237431
H	0.479015	-5.190211	-3.073433
H	2.558423	-4.414190	0.661620
H	2.414402	-5.618588	-1.536895
C	-2.975067	-2.988015	0.782316
C	-4.162011	-2.397511	1.276964
C	-2.778031	-4.374397	0.952013
C	-5.135523	-3.178807	1.916726
H	-4.324973	-1.314261	1.157826
C	-3.748181	-5.152191	1.610569
H	-1.860749	-4.851673	0.574231
C	-4.927571	-4.560477	2.091902
H	-6.057618	-2.705431	2.290119
H	-3.576959	-6.232271	1.744203
H	-5.685628	-5.172962	2.605317
C	-1.154706	3.470899	1.268364
C	-2.152789	4.431639	1.536599
C	0.095909	3.566369	1.927503
C	-1.898094	5.477193	2.443359

H	-3.129701	4.368920	1.031805
C	0.349340	4.620653	2.817209
H	0.875063	2.813579	1.725547
C	-0.649377	5.578180	3.080639
H	-2.682962	6.223742	2.645712
H	1.331220	4.690547	3.311905
H	-0.452783	6.402632	3.784312
C	-3.039309	2.314460	-0.633246
C	-3.191919	3.317336	-1.617115
C	-4.136983	1.494728	-0.303931
C	-4.428828	3.494053	-2.256592
H	-2.333977	3.952605	-1.889914
C	-5.373247	1.670048	-0.948156
H	-4.007010	0.698935	0.447079
C	-5.520022	2.668714	-1.925899
H	-4.540150	4.275876	-3.024973
H	-6.219785	1.011950	-0.696568
H	-6.485905	2.800544	-2.439164
H	-2.515636	-0.170278	2.091114
C	-0.658175	0.517858	3.519871
C	-1.907516	-0.159320	3.612372
H	-2.792213	0.483615	3.789671
H	-0.630109	1.620112	3.553771
H	0.260097	-0.000207	3.844748
C	-2.033315	-1.569443	4.152921
H	-2.191830	-1.528933	5.253510
H	-2.897281	-2.106349	3.712909
H	-1.121085	-2.164665	3.950612

IM6

Free Energy **=** -3206.260733

Energy = -3207.055915

B	-3.751890	-0.497735	0.278703
C	-4.051139	0.764167	-0.729055
C	-3.034149	1.200855	-1.613776
C	-5.314217	1.384476	-0.844672
C	-3.271610	2.181985	-2.587593
H	-2.029015	0.756903	-1.535738
C	-5.563408	2.378029	-1.813896
H	-6.128687	1.074842	-0.167939
C	-4.545300	2.773920	-2.696991
H	-2.455552	2.496616	-3.259048
H	-6.563021	2.839887	-1.882806
H	-4.737698	3.546529	-3.459977
C	-3.350692	-1.816741	-0.625256
C	-4.071836	-2.101259	-1.811681
C	-2.312202	-2.716806	-0.284863
C	-3.786597	-3.227166	-2.606003
H	-4.873343	-1.411766	-2.126887
C	-2.010809	-3.840197	-1.074922
H	-1.716270	-2.537388	0.624227
C	-2.750326	-4.104863	-2.240873
H	-4.372460	-3.415483	-3.521648
H	-1.192212	-4.518374	-0.780107
H	-2.513919	-4.981971	-2.865288
C	-4.979019	-0.760250	1.321832
C	-5.127956	0.057242	2.469652
C	-5.979353	-1.733889	1.097546
C	-6.213534	-0.086934	3.351281
H	-4.368741	0.832728	2.674762
C	-7.074521	-1.886438	1.969079
H	-5.897843	-2.394073	0.217618
C	-7.196321	-1.063306	3.102607
H	-6.296839	0.565307	4.237189
H	-7.836740	-2.657062	1.763772
H	-8.050927	-1.182228	3.789068
C	-1.361726	-0.022616	1.457825
N	-2.473640	-0.145748	1.089336
P	2.157954	-1.328812	-0.170028
C	1.298756	-1.750193	-1.768192
O	0.279592	0.460710	-1.900813
C	1.364758	1.271578	-2.204406
C	1.992396	1.230865	-3.459787
C	3.102084	2.057355	-3.693546
C	3.583196	2.906091	-2.680951
C	2.937237	2.950168	-1.434434
C	1.811670	2.140805	-1.183569
C	1.443983	-3.014074	-2.386233
C	0.619770	-3.399469	-3.455608
C	-0.389564	-2.537666	-3.915109
C	-0.511189	-1.251965	-3.367106
C	0.357507	-0.854848	-2.342616
P	0.896172	2.015249	0.403856
Pd	0.573383	-0.242178	1.202593
H	1.620142	0.541957	-4.232337
H	3.605090	2.023996	-4.672667
H	4.472549	3.530083	-2.856971
H	3.328956	3.599562	-0.637242
H	2.198821	-3.720338	-2.011133
H	0.748511	-4.394781	-3.907995
H	-1.077118	-2.856611	-4.712451
H	-1.264807	-0.535850	-3.725260
C	-0.573198	3.091929	0.108112
C	-0.678164	3.917094	-1.032656
C	-1.614987	3.089228	1.060624
C	-1.818986	4.714734	-1.219687
H	0.123260	3.928575	-1.787419
C	-2.760558	3.873751	0.857418
H	-1.542458	2.457034	1.958095
C	-2.866662	4.685221	-0.284690
H	-1.901132	5.342724	-2.120834
H	-3.582988	3.833847	1.588118
H	-3.777096	5.279767	-0.455872
C	1.878444	2.992064	1.622541
C	2.463520	2.326715	2.722260
C	2.024340	4.392324	1.501303
C	3.214984	3.044585	3.668410
H	2.309601	1.240048	2.847790
C	2.780710	5.105963	2.445290
H	1.532450	4.926257	0.672227
C	3.381558	4.433174	3.525574
H	3.663258	2.517004	4.525162
H	2.893443	6.197019	2.342551
H	3.968638	4.997229	4.267806

C	2.777163	-2.963527	0.432270
C	4.086445	-3.098466	0.944612
C	1.891176	-4.065199	0.516620
C	4.498429	-4.308725	1.528904
H	4.794273	-2.257008	0.888474
C	2.312707	-5.275579	1.089083
H	0.869687	-3.983337	0.115074
C	3.615528	-5.399408	1.602843
H	5.522903	-4.398041	1.923741
H	1.610894	-6.122700	1.141262
H	3.942254	-6.346555	2.060313
C	3.715807	-0.449135	-0.612452
C	4.343414	-0.611841	-1.863579
C	4.316389	0.365881	0.370615
C	5.564652	0.033107	-2.121505
H	3.868672	-1.232636	-2.639766
C	5.542029	0.999816	0.113348
H	3.814765	0.513192	1.338810
C	6.167962	0.833041	-1.134535
H	6.045502	-0.085656	-3.105385
H	5.998917	1.637204	0.886635
H	7.124141	1.338381	-1.344173
H	1.464711	-0.969484	4.086881
C	0.400755	-1.931695	2.448828
C	1.567586	-1.865940	3.434224
H	2.539244	-1.757974	2.901150
H	0.413590	-2.860704	1.849347
H	-0.569386	-1.894492	2.982769
C	1.642671	-3.132126	4.309026
H	2.472966	-3.070629	5.045125
H	0.699337	-3.289811	4.874316
H	1.814763	-4.029985	3.678665

TS3'

Free Energy = -3206.24329

Energy = -3207.033466

B	3.646811	0.108913	-0.047771
C	3.594200	-0.048290	1.583288
C	2.582683	-0.800721	2.228163
C	4.575330	0.542955	2.414163
C	2.537574	-0.945826	3.625738
H	1.791042	-1.280356	1.627491
C	4.546332	0.402586	3.814613
H	5.376006	1.143815	1.951320
C	3.520995	-0.339066	4.428410
H	1.725976	-1.529363	4.086026
H	5.324533	0.883181	4.431135
H	3.487272	-0.443839	5.525409
C	4.237524	-1.227545	-0.793547
C	4.964705	-2.228061	-0.109811
C	4.058593	-1.406410	-2.188656
C	5.497718	-3.347454	-0.780467
H	5.117537	-2.128552	0.978130
C	4.580273	-2.519041	-2.870319
H	3.495472	-0.644821	-2.755728
C	5.308576	-3.497419	-2.165767
H	6.061937	-4.108786	-0.216009
H	4.419087	-2.627178	-3.956031
H	5.721320	-4.372831	-2.693571
C	4.421833	1.484146	-0.481666
C	3.809437	2.744099	-0.264092
C	5.733379	1.487811	-1.007668
C	4.469804	3.948614	-0.559785
H	2.789313	2.781108	0.157321
C	6.408182	2.688788	-1.303282
H	6.241178	0.525287	-1.190160
C	5.777306	3.925505	-1.082400
H	3.964001	4.912018	-0.378085
H	7.432936	2.658215	-1.710700
H	6.301432	4.867451	-1.314788
C	1.060338	0.325034	-0.867409
N	2.184020	0.251891	-0.532841
P	-1.442953	-1.805968	-0.097055
C	-1.126602	-2.003325	1.729656
O	-1.860638	0.274304	2.168067
C	-3.138199	0.467802	1.695871
C	-4.239287	-0.267278	2.165213
C	-5.507692	-0.018837	1.620350
C	-5.665164	0.950724	0.614759
C	-4.554280	1.677035	0.152129
C	-3.269108	1.461113	0.696356
C	-0.604622	-3.199070	2.276267
C	-0.419032	-3.351357	3.660059
C	-0.740851	-2.299165	4.534714
C	-1.241004	-1.094585	4.017833
C	-1.436684	-0.957968	2.634529
P	-1.706338	2.081952	-0.082564
Pd	-0.856852	0.297522	-1.401492
H	-4.086686	-1.042039	2.931166
H	-6.372138	-0.603900	1.969663
H	-6.655910	1.131462	0.169982
H	-4.688804	2.398000	-0.668097
H	-0.336869	-4.026371	1.601581
H	-0.011596	-4.295635	4.052943
H	-0.586756	-2.407677	5.619548
H	-1.481094	-0.239551	4.666699
C	-0.574041	2.808750	1.201715
C	0.406808	1.983246	1.797193
C	-0.588741	4.186067	1.516746
C	1.345516	2.516003	2.692567
H	0.455639	0.914248	1.556384
C	0.353585	4.717908	2.415112
H	-1.320936	4.862182	1.051534
C	1.322374	3.887271	3.002816
H	2.107730	1.852688	3.129263
H	0.332396	5.795305	2.645284
H	2.069561	4.308541	3.694017
C	-2.219166	3.558162	-1.063881
C	-1.555725	3.786940	-2.289083
C	-3.175677	4.497888	-0.612271
C	-1.850001	4.926181	-3.057301
H	-0.792660	3.066830	-2.628278
C	-3.474430	5.630902	-1.387494
H	-3.686979	4.349688	0.351809
C	-2.814685	5.846081	-2.611132

H	-1.320179	5.095360	-4.008155
H	-4.223238	6.354824	-1.028305
H	-3.049623	6.736926	-3.215182
C	-0.474849	-3.219653	-0.777818
C	-1.064630	-4.286801	-1.488071
C	0.935652	-3.147814	-0.679181
C	-0.251108	-5.260399	-2.097097
H	-2.160237	-4.353836	-1.577012
C	1.741211	-4.131053	-1.269650
H	1.419074	-2.311790	-0.152132
C	1.148423	-5.186141	-1.989286
H	-0.719688	-6.085527	-2.657587
H	2.835804	-4.052934	-1.182696
H	1.782086	-5.949639	-2.468011
C	-3.208978	-2.367831	-0.194009
C	-3.697551	-3.432075	0.599573
C	-4.096108	-1.696036	-1.057413
C	-5.046686	-3.810957	0.523546
H	-3.022311	-3.962370	1.289084
C	-5.445820	-2.078750	-1.136378
H	-3.730852	-0.839370	-1.645260
C	-5.924441	-3.136040	-0.345784
H	-5.416792	-4.638254	1.150167
H	-6.128673	-1.532960	-1.806272
H	-6.984465	-3.431463	-0.399244
H	-2.309762	0.352325	-2.077863
C	-1.555348	0.218340	-3.591702
C	-0.222457	-0.251624	-3.508699
H	0.578642	0.491514	-3.673765
H	-1.758079	1.255918	-3.906307
H	-2.351860	-0.506071	-3.842835
C	0.168493	-1.688518	-3.726459
H	1.065464	-1.964293	-3.137568
H	-0.646889	-2.389805	-3.461815
H	0.421795	-1.844731	-4.800186

IM6'

Free Energy = -3206.249762

Energy = -3207.041407

B	3.699011	0.040140	-0.059307
C	3.565202	-0.155277	1.563951
C	2.486327	-0.866377	2.143007
C	4.542119	0.351433	2.453522
C	2.372551	-1.051627	3.531460
H	1.694187	-1.279153	1.495869
C	4.446648	0.168267	3.846427
H	5.395437	0.917189	2.043580
C	3.355756	-0.530818	4.393273
H	1.507980	-1.597512	3.938546
H	5.225159	0.581881	4.509406
H	3.269870	-0.667994	5.483844
C	4.200500	-1.329633	-0.810449
C	4.893590	-2.356760	-0.129583
C	3.992575	-1.511577	-2.200991
C	5.365510	-3.503864	-0.798372
H	5.067576	-2.256229	0.955057
C	4.452797	-2.652710	-2.880719
H	3.455303	-0.730629	-2.766690
C	5.147584	-3.656960	-2.179271
H	5.903755	-4.285164	-0.235843
H	4.269643	-2.761929	-3.962856
H	5.511696	-4.554623	-2.705492
C	4.611360	1.348292	-0.428922
C	4.136654	2.646158	-0.111464
C	5.895316	1.256071	-1.010568
C	4.901635	3.796492	-0.367025
H	3.142108	2.753769	0.357036
C	6.674751	2.401678	-1.266986
H	6.295651	0.261467	-1.271350
C	6.179328	3.677865	-0.948055
H	4.503056	4.792204	-0.108619
H	7.674574	2.296643	-1.721332
H	6.785103	4.577025	-1.149295
C	1.168698	0.455209	-0.980632
N	2.273884	0.322956	-0.599499
P	-1.551503	-1.728199	-0.103123
C	-1.290864	-1.929208	1.737761
O	-1.949714	0.373657	2.163191
C	-3.200613	0.605798	1.639118
C	-4.348989	-0.075068	2.072727
C	-5.582005	0.221208	1.471446
C	-5.656602	1.182762	0.448498
C	-4.497838	1.855004	0.021980
C	-3.247333	1.587401	0.621029
C	-0.828364	-3.143220	2.298295
C	-0.685252	-3.302647	3.686636
C	-0.989475	-2.239706	4.554239
C	-1.430197	-1.017578	4.024688
C	-1.583585	-0.874071	2.636721
P	-1.617063	2.117253	-0.071352
Pd	-0.725882	0.343404	-1.422532
H	-4.261636	-0.844452	2.854215
H	-6.484928	-0.321217	1.790931
H	-6.620419	1.399274	-0.037476
H	-4.567137	2.574193	-0.808090
H	-0.573126	-3.981283	1.632335
H	-0.322779	-4.261628	4.087850
H	-0.867587	-2.353748	5.642567
H	-1.655970	-0.153613	4.666855
C	-0.529701	2.807657	1.264137
C	0.446805	1.956216	1.827206
C	-0.567904	4.163525	1.655653
C	1.366101	2.445172	2.766851
H	0.499048	0.901358	1.527148
C	0.352952	4.651155	2.599995
H	-1.299109	4.857374	1.215378
C	1.321382	3.796433	3.154157
H	2.126516	1.765365	3.180447
H	0.316847	5.712734	2.893144
H	2.051525	4.184662	3.882088
C	-2.009387	3.592055	-1.110225
C	-1.303580	3.749770	-2.323828
C	-2.930397	4.591414	-0.715134
C	-1.519185	4.878840	-3.132350
H	-0.570646	2.981124	-2.623466

C	-3.146788	5.716120	-1.528465
H	-3.483399	4.493272	0.232129
C	-2.443806	5.861392	-2.738308
H	-0.957779	4.991464	-4.073395
H	-3.867220	6.487053	-1.211558
H	-2.615297	6.745678	-3.372559
C	-0.622582	-3.200090	-0.713574
C	-1.232914	-4.341505	-1.274786
C	0.789325	-3.116726	-0.671289
C	-0.435972	-5.381288	-1.789676
H	-2.330427	-4.418748	-1.320920
C	1.579130	-4.164381	-1.163892
H	1.283265	-2.217222	-0.274153
C	0.966188	-5.297132	-1.732147
H	-0.918910	-6.265793	-2.235782
H	2.675668	-4.078179	-1.121639
H	1.586367	-6.113758	-2.134966
C	-3.336653	-2.213108	-0.239344
C	-3.922631	-3.207939	0.577199
C	-4.142608	-1.529559	-1.172205
C	-5.287509	-3.511338	0.453518
H	-3.309804	-3.740741	1.321340
C	-5.507811	-1.837497	-1.298406
H	-3.704746	-0.724276	-1.780493
C	-6.083013	-2.828013	-0.485819
H	-5.735506	-4.285135	1.097471
H	-6.127219	-1.285056	-2.022361
H	-7.155412	-3.063821	-0.576211
H	-2.178071	0.470180	-2.621137
C	-1.642167	0.112657	-3.618367
C	-0.247361	-0.362873	-3.372662
H	0.537157	0.336734	-3.717027
H	-1.726891	1.012014	-4.260090
H	-2.330116	-0.688463	-3.959185
C	0.104881	-1.803431	-3.636222
H	1.077686	-2.074114	-3.180879
H	-0.661729	-2.509424	-3.259779
H	0.199722	-1.966149	-4.736019

TS4

Free Energy = -3206.25416

Energy = -3207.047903

B	3.945096	0.582104	-0.042999
C	4.614646	1.511022	-1.231973
C	4.272251	2.885216	-1.309335
C	5.514373	1.018101	-2.202427
C	4.789414	3.724942	-2.309874
H	3.587955	3.306414	-0.551432
C	6.047742	1.851497	-3.206311
H	5.804273	-0.045825	-2.173521
C	5.683719	3.207514	-3.267509
H	4.502743	4.789915	-2.341521
H	6.751935	1.437027	-3.947642
H	6.097193	3.860937	-4.053572
C	4.293658	1.235248	1.416035
C	5.643219	1.496225	1.763037
C	3.314911	1.592419	2.372617
C	5.999589	2.047334	3.006359
H	6.435490	1.274872	1.027533
C	3.655042	2.156324	3.617527
H	2.250566	1.425625	2.138345
C	5.003962	2.379241	3.944528
H	7.061239	2.231580	3.242319
H	2.861382	2.425997	4.335128
H	5.278447	2.818683	4.917689
C	4.349883	-1.002303	-0.193874
C	3.735345	-1.784089	-1.203971
C	5.341317	-1.645565	0.581526
C	4.085700	-3.123920	-1.439071
H	2.955410	-1.323492	-1.831298
C	5.716264	-2.983224	0.349835
H	5.831269	-1.089770	1.397943
C	5.090366	-3.730795	-0.663239
H	3.567220	-3.695151	-2.227780
H	6.496179	-3.449275	0.975619
H	5.376951	-4.780591	-0.841168
C	1.273973	0.842123	-0.519783
N	2.426411	0.698591	-0.271965
P	-2.914965	1.088114	-0.155846
C	-4.257014	0.384871	-1.223479
O	-3.188811	-1.784738	-1.048511
C	-3.233051	-2.257673	0.251660
C	-4.432527	-2.491370	0.940408
C	-4.377380	-2.996042	2.250780
C	-3.140431	-3.275269	2.857669
C	-1.945090	-3.018722	2.164894
C	-1.975845	-2.489241	0.859214
C	-5.307669	1.156973	-1.766943
C	-6.275180	0.573194	-2.602307
C	-6.205484	-0.795597	-2.914612
C	-5.175432	-1.584980	-2.377976
C	-4.221103	-0.997394	-1.533439
P	-0.502248	-1.813964	-0.004431
Pd	-0.616868	0.471736	-0.484072
H	-5.394919	-2.266245	0.457623
H	-5.315369	-3.169366	2.800907
H	-3.104324	-3.674625	3.882822
H	-0.973011	-3.198022	2.650765
H	-5.363507	2.232763	-1.539758
H	-7.084822	1.195069	-3.014857
H	-6.956109	-1.253951	-3.577396
H	-5.091956	-2.659286	-2.600381
C	-0.275020	-2.881986	-1.484609
C	0.425021	-2.360503	-2.592982
C	-0.734906	-4.215951	-1.511752
C	0.687625	-3.174728	-3.706923
H	0.761620	-1.311343	-2.581182
C	-0.477597	-5.024231	-2.632006
H	-1.289798	-4.623679	-0.651337
C	0.239433	-4.507898	-3.726628
H	1.243438	-2.762901	-4.563970
H	-0.835796	-6.066059	-2.647624
H	0.444635	-5.145434	-4.601401
C	0.903232	-2.243202	1.100527
C	1.257257	-1.320868	2.109361

C	1.646506	-3.434101	0.956833
C	2.331400	-1.588120	2.970785
H	0.705253	-0.371135	2.197849
C	2.718559	-3.699321	1.823213
H	1.409043	-4.145461	0.151750
C	3.064549	-2.777964	2.825764
H	2.620403	-0.847091	3.730938
H	3.310989	-4.616448	1.687369
H	3.928480	-2.974467	3.479491
C	-3.104730	2.907994	-0.363012
C	-3.243487	3.776593	0.741066
C	-2.938431	3.456212	-1.658385
C	-3.227868	5.169340	0.548997
H	-3.361343	3.365438	1.755762
C	-2.942056	4.847422	-1.845183
H	-2.820890	2.788992	-2.528545
C	-3.083081	5.707876	-0.740996
H	-3.333918	5.838207	1.417780
H	-2.820905	5.261421	-2.858656
H	-3.071689	6.799365	-0.886918
C	-3.543014	0.753357	1.547347
C	-4.913276	0.878182	1.866326
C	-2.626317	0.368210	2.546846
C	-5.355833	0.621151	3.172998
H	-5.636550	1.168812	1.087735
C	-3.073952	0.106898	3.852659
H	-1.560824	0.252388	2.290200
C	-4.437380	0.233735	4.167008
H	-6.425926	0.717474	3.416766
H	-2.352945	-0.209247	4.622450
H	-4.788752	0.023558	5.189765
C	0.425443	2.494809	-1.059548
C	0.544601	3.486615	0.093087
H	1.433728	3.235402	0.711609
H	1.241521	2.595729	-1.801735
H	-0.523734	2.618457	-1.624365
H	-0.341787	3.393205	0.757806
C	0.661672	4.929039	-0.418346
H	0.730100	5.649743	0.423837
H	1.569786	5.056996	-1.046023
H	-0.219215	5.212163	-1.031897

IM7

Free Energy **=** -3206.261732

Energy = -3207.056443

B	3.825166	0.655954	-0.032258
C	4.157018	-0.782029	-0.758920
C	4.079553	-2.022841	-0.087999
C	4.465563	-0.823686	-2.142247
C	4.311676	-3.242929	-0.750215
H	3.825663	-2.037640	0.982027
C	4.708754	-2.034325	-2.815267
H	4.531274	0.123725	-2.703908
C	4.634625	-3.254488	-2.117593
H	4.231361	-4.190403	-0.192245
H	4.958578	-2.026936	-3.889792
H	4.816199	-4.207696	-2.640577
C	4.789972	1.863875	-0.611198
C	6.173064	1.632551	-0.809788
C	4.322810	3.174867	-0.857845
C	7.043007	2.652028	-1.233948
H	6.577599	0.621589	-0.632670
C	5.180784	4.205079	-1.286796
H	3.256590	3.403136	-0.700738
C	6.549366	3.947251	-1.478996
H	8.114959	2.434863	-1.377580
H	4.778355	5.216012	-1.469902
H	7.227496	4.748786	-1.815287
C	3.987908	0.696703	1.597048
C	5.075872	0.060030	2.240442
C	3.119412	1.455792	2.416938
C	5.274883	0.152264	3.629382
H	5.786341	-0.529200	1.636983
C	3.308274	1.562604	3.806947
H	2.265196	1.980988	1.954283
C	4.388396	0.903541	4.423463
H	6.129751	-0.364358	4.097188
H	2.609023	2.162068	4.414086
H	4.541006	0.978913	5.512628
C	1.244681	1.204125	-0.751139
N	2.368252	0.968878	-0.390111
P	-2.901480	1.129841	-0.045206
C	-4.200443	0.515622	-1.217131
O	-3.072696	-1.641691	-1.283462
C	-3.146809	-2.186474	-0.011637
C	-4.377970	-2.456628	0.608410
C	-4.392074	-3.039584	1.885111
C	-3.185349	-3.364847	2.526222
C	-1.960422	-3.082159	1.900476
C	-1.916275	-2.472763	0.628207
C	-5.260421	1.317011	-1.697711
C	-6.167676	0.824072	-2.650610
C	-6.026359	-0.482826	-3.149026
C	-4.990111	-1.303993	-2.675715
C	-4.097890	-0.810276	-1.711673
P	-0.356985	-1.802922	-0.108556
Pd	-0.639115	0.449375	-0.522337
H	-5.315211	-2.196121	0.094943
H	-5.355945	-3.236136	2.379753
H	-3.194018	-3.822870	3.527113
H	-1.019212	-3.308996	2.423080
H	-5.367458	2.349483	-1.330125
H	-6.985115	1.468960	-3.009194
H	-6.728023	-0.869250	-3.904803
H	-4.856101	-2.335096	-3.035488
C	-0.013520	-2.844799	-1.585337
C	1.132257	-2.526872	-2.349439
C	-0.848302	-3.910883	-1.981433
C	1.431042	-3.270817	-3.501263
H	1.802164	-1.708019	-2.036596
C	-0.544085	-4.647716	-3.139225
H	-1.735240	-4.169779	-1.382560
C	0.592492	-4.327287	-3.902178
H	2.331373	-3.020825	-4.082578
H	-1.200084	-5.478958	-3.444507

H	0.827848	-4.904559	-4.810759
C	0.893130	-2.334975	1.125977
C	1.310387	-1.408403	2.102210
C	1.370951	-3.663811	1.167434
C	2.188285	-1.807338	3.124407
H	0.970775	-0.362260	2.045724
C	2.242363	-4.060341	2.193858
H	1.061997	-4.384850	0.394130
C	2.649643	-3.133691	3.173414
H	2.540482	-1.065546	3.857279
H	2.616827	-5.096088	2.222895
H	3.349569	-3.441365	3.966313
C	-3.079866	2.959984	-0.123114
C	-3.176650	3.745837	1.046536
C	-2.937607	3.602510	-1.377636
C	-3.133339	5.148602	0.960459
H	-3.280361	3.261319	2.030138
C	-2.918389	5.002949	-1.457859
H	-2.851285	3.001424	-2.297926
C	-3.008023	5.781262	-0.288302
H	-3.204128	5.750578	1.880489
H	-2.822649	5.491749	-2.440328
H	-2.978011	6.880331	-0.352049
C	-3.569568	0.675199	1.613131
C	-4.945570	0.777843	1.914869
C	-2.671603	0.210473	2.595743
C	-5.413544	0.418803	3.188305
H	-5.653383	1.131276	1.148231
C	-3.144726	-0.148586	3.869560
H	-1.601646	0.108393	2.350537
C	-4.513850	-0.045197	4.166777
H	-6.488278	0.496416	3.418261
H	-2.438222	-0.524604	4.625925
H	-4.884782	-0.334445	5.163044
C	0.580274	2.422318	-1.451027
C	0.538381	3.687349	-0.565381
H	1.385762	3.658768	0.152857
H	1.231799	2.564139	-2.340229
H	-0.436195	2.229396	-1.882250
H	-0.388068	3.671336	0.046539
C	0.609598	4.967703	-1.400709
H	-0.192727	4.996493	-2.166858
H	0.494398	5.869173	-0.764325
H	1.584103	5.047198	-1.929323

TS5

Free Energy = -3206.259044

Energy = -3207.053738

B	3.446974	0.998363	-0.279186
C	3.629870	-0.409813	-1.077012
C	3.827542	-1.649149	-0.432654
C	3.737293	-0.391360	-2.491721
C	4.122469	-2.817657	-1.162223
H	3.749982	-1.708193	0.664237
C	4.031291	-1.549683	-3.229147
H	3.606178	0.564508	-3.028583
C	4.226499	-2.773873	-2.561650
H	4.263337	-3.769369	-0.626168
H	4.109384	-1.500417	-4.328086
H	4.449431	-3.689719	-3.132447
C	4.804716	1.919701	-0.435014
C	6.068986	1.315433	-0.631400
C	4.780676	3.328017	-0.297436
C	7.251995	2.076479	-0.679902
H	6.129416	0.221219	-0.753248
C	5.953753	4.100276	-0.356952
H	3.818850	3.840340	-0.130603
C	7.199644	3.474877	-0.546655
H	8.221448	1.572436	-0.829837
H	5.897497	5.196588	-0.249544
H	8.123750	4.074285	-0.591163
C	3.027295	0.928213	1.305305
C	4.005709	0.539364	2.253256
C	1.765318	1.308393	1.819790
C	3.739023	0.526362	3.633088
H	5.011653	0.257069	1.900577
C	1.486724	1.313078	3.199947
H	0.940088	1.598890	1.133509
C	2.477001	0.920593	4.116665
H	4.526350	0.213929	4.338822
H	0.489253	1.622228	3.554186
H	2.269825	0.924271	5.199187
C	1.422647	2.488377	-1.293313
N	2.302772	1.790790	-0.967299
P	-2.501892	1.184497	-0.258384
C	-3.802949	0.360968	-1.333287
O	-2.730140	-1.796055	-1.020431
C	-2.840527	-2.225343	0.287400
C	-4.076417	-2.372796	0.936456
C	-4.102995	-2.848830	2.257884
C	-2.906331	-3.189781	2.909854
C	-1.675016	-3.024143	2.251842
C	-1.616452	-2.515986	0.937868
C	-4.872695	1.066097	-1.934327
C	-5.801696	0.424571	-2.770583
C	-5.683304	-0.950467	-3.034022
C	-4.648414	-1.681063	-2.431360
C	-3.736769	-1.033833	-1.580711
P	-0.054520	-1.978676	0.087804
Pd	-0.399678	0.307100	-0.309248
H	-5.004413	-2.103061	0.411206
H	-5.068898	-2.949649	2.776909
H	-2.926016	-3.571219	3.942575
H	-0.740954	-3.270548	2.779305
H	-4.984136	2.144835	-1.750734
H	-6.619926	1.008472	-3.220668
H	-6.399616	-1.457401	-3.699554
H	-4.527573	-2.762012	-2.597483
C	-0.009532	-3.026000	-1.433244
C	0.803428	-2.587536	-2.497286
C	-0.740280	-4.227013	-1.564452
C	0.894804	-3.345856	-3.676400
H	1.377367	-1.652632	-2.394137
C	-0.654708	-4.977894	-2.748724
H	-1.378523	-4.575061	-0.736075

C	0.163575	-4.539450	-3.806878
H	1.545705	-2.998002	-4.493982
H	-1.229691	-5.913211	-2.845957
H	0.230116	-5.130338	-4.734738
C	1.199409	-2.792657	1.180083
C	1.575897	-2.116749	2.360331
C	1.771404	-4.050040	0.892156
C	2.506610	-2.689728	3.241946
H	1.149855	-1.127222	2.583931
C	2.714938	-4.613342	1.768101
H	1.494443	-4.584499	-0.029149
C	3.086201	-3.935624	2.943577
H	2.790100	-2.144664	4.154969
H	3.166234	-5.589490	1.527052
H	3.829520	-4.378251	3.625969
C	-2.930746	2.966848	-0.560906
C	-3.255867	3.863792	0.480679
C	-2.806134	3.474336	-1.878305
C	-3.455093	5.229705	0.210560
H	-3.352859	3.494964	1.513670
C	-3.017951	4.835386	-2.147573
H	-2.564507	2.787256	-2.707289
C	-3.339554	5.721486	-1.101237
H	-3.707487	5.914265	1.036340
H	-2.929169	5.207479	-3.180991
H	-3.500771	6.790878	-1.310216
C	-3.226543	0.884858	1.430336
C	-4.610287	1.019065	1.680165
C	-2.371283	0.479013	2.475878
C	-5.125840	0.754626	2.958915
H	-5.290060	1.323635	0.868278
C	-2.890320	0.210181	3.753579
H	-1.296222	0.343245	2.264761
C	-4.267081	0.348529	3.997547
H	-6.207084	0.857838	3.144756
H	-2.213621	-0.124170	4.555599
H	-4.675811	0.129931	4.997161
C	0.538900	3.609051	-1.579662
C	0.108721	4.322138	-0.272423
H	-0.596325	5.123698	-0.575048
H	1.095338	4.300299	-2.252682
H	-0.350397	3.245774	-2.131016
H	-0.481652	3.602652	0.330896
C	1.260457	4.885495	0.559094
H	1.908579	4.078978	0.961431
H	1.896148	5.582435	-0.027683
H	0.865999	5.446072	1.431268

IM8

Free Energy = -3206.27743

Energy = -3207.073465

B	-3.207822	-0.809311	-0.112435
C	-2.200665	-0.740454	-1.402517
C	-2.492771	0.147200	-2.492806
C	-1.317734	-1.847673	-1.692384
C	-1.963146	-0.040954	-3.770168
H	-3.187945	0.983418	-2.318295
C	-0.805612	-2.049105	-3.015874
H	-1.282063	-2.697205	-0.989580
C	-1.111943	-1.149834	-4.035424
H	-2.215948	0.664460	-4.578330
H	-0.171790	-2.927016	-3.219886
H	-0.710244	-1.307453	-5.050043
C	-4.527653	-1.736462	-0.423187
C	-4.743909	-2.365608	-1.669784
C	-5.513476	-1.926100	0.576851
C	-5.891099	-3.146183	-1.911794
H	-4.001034	-2.240498	-2.474967
C	-6.658873	-2.707615	0.350095
H	-5.383541	-1.434786	1.557272
C	-6.852117	-3.322743	-0.901535
H	-6.033897	-3.620438	-2.897208
H	-7.409126	-2.834118	1.148737
H	-7.750729	-3.933675	-1.087919
C	-3.607439	0.650988	0.499875
C	-4.729147	1.342949	-0.019094
C	-2.853805	1.308172	1.502297
C	-5.074395	2.631914	0.427479
H	-5.348978	0.855907	-0.790175
C	-3.206465	2.584395	1.976123
H	-1.948603	0.829124	1.912381
C	-4.315604	3.256452	1.433456
H	-5.947082	3.147888	-0.006423
H	-2.598233	3.061025	2.760279
H	-4.586369	4.263206	1.790840
C	-1.960404	-2.017551	1.992785
N	-2.457453	-1.550916	1.048933
P	0.445431	1.999764	-0.274522
C	0.581631	2.544470	1.500452
O	1.660460	0.442367	2.119378
C	2.970404	0.401941	1.659752
C	3.976533	1.179951	2.256427
C	5.287832	1.109921	1.761362
C	5.584057	0.271933	0.673265
C	4.574244	-0.518238	0.099763
C	3.250656	-0.482398	0.589578
C	0.018699	3.759041	1.956650
C	-0.038329	4.076022	3.324577
C	0.454076	3.172157	4.280486
C	1.032387	1.964269	3.855472
C	1.110773	1.667989	2.485627
P	1.846304	-1.427940	-0.161871
Pd	-0.078532	-0.236646	-0.646070
H	3.720546	1.850977	3.089771
H	6.076306	1.726224	2.221438
H	6.605399	0.232150	0.264088
H	4.813512	-1.167322	-0.755936
H	-0.406543	4.460372	1.222861
H	-0.487320	5.030093	3.642522
H	0.396195	3.405634	5.355239
H	1.439302	1.236033	4.573065
C	1.652332	-2.847525	1.015817
C	0.844003	-3.932924	0.593662
C	2.251922	-2.905170	2.293252
C	0.658726	-5.053397	1.417893

H	0.379854	-3.908396	-0.405035
C	2.061771	-4.028778	3.119044
H	2.892497	-2.080253	2.640472
C	1.267676	-5.106691	2.687660
H	0.036277	-5.891741	1.066286
H	2.555140	-4.067696	4.103534
H	1.126222	-5.986848	3.334577
C	2.674423	-2.279234	-1.584624
C	2.485780	-1.735945	-2.874064
C	3.475384	-3.434926	-1.435311
C	3.097266	-2.326602	-3.993121
H	1.837545	-0.856453	-2.995510
C	4.080367	-4.027401	-2.556080
H	3.629678	-3.871170	-0.435597
C	3.894938	-3.473433	-3.836965
H	2.937190	-1.893576	-4.993553
H	4.703402	-4.927386	-2.428401
H	4.369118	-3.941672	-4.714543
C	-0.472880	3.422428	-1.040843
C	0.166820	4.587407	-1.524085
C	-1.873516	3.309772	-1.155989
C	-0.590531	5.621525	-2.100411
H	1.261140	4.688881	-1.452172
C	-2.629112	4.347920	-1.724531
H	-2.369033	2.400012	-0.793495
C	-1.989765	5.506190	-2.199811
H	-0.082577	6.524374	-2.476851
H	-3.723040	4.240235	-1.794594
H	-2.579711	6.318724	-2.654057
C	2.139057	2.301728	-0.964032
C	3.161657	2.999490	-0.292421
C	2.392880	1.777704	-2.251309
C	4.430409	3.136220	-0.884090
H	2.972018	3.426750	0.704437
C	3.655761	1.921668	-2.844100
H	1.582776	1.252498	-2.783973
C	4.682588	2.593393	-2.155365
H	5.229763	3.663805	-0.339927
H	3.842237	1.496681	-3.843265
H	5.680943	2.692779	-2.610628
C	-1.312783	-2.450202	3.215958
C	-0.540032	-1.281010	3.877213
H	-1.228870	-0.422056	4.023476
H	-2.099073	-2.856742	3.890392
H	-0.627098	-3.290549	2.972151
H	0.245739	-0.945907	3.170549
C	0.077040	-1.702322	5.210562q
H	0.644480	-0.862981	5.663024
H	-0.697276	-2.014555	5.943622
H	0.779565	-2.550794	5.078781

TS3-b

Free Energy = -3437.334579

Energy = -3438.198879

B	-3.623460	-0.775029	-0.509671
C	-4.049107	-0.614101	1.063957
C	-3.309390	-1.290291	2.063809
C	-5.173868	0.126411	1.491036
C	-3.672478	-1.244874	3.419603
H	-2.421731	-1.864253	1.765893
C	-5.546796	0.189351	2.848703
H	-5.772013	0.673928	0.743278
C	-4.798251	-0.498911	3.820954
H	-3.067623	-1.787075	4.165510
H	-6.430215	0.777820	3.149240
H	-5.089695	-0.455028	4.883499
C	-4.326198	0.347313	-1.469731
C	-3.946224	1.706508	-1.335724
C	-5.314492	0.048417	-2.432803
C	-4.508353	2.718701	-2.131306
H	-3.190151	1.975157	-0.579583
C	-5.894433	1.054666	-3.231521
H	-5.634398	-0.999342	-2.565999
C	-5.490048	2.393873	-3.088242
H	-4.181108	3.764550	-2.002611
H	-6.664124	0.789722	-3.976085
H	-5.938682	3.181208	-3.716545
C	-3.821865	-2.322729	-1.023540
C	-3.067854	-2.838858	-2.106490
C	-4.732121	-3.209734	-0.403186
C	-3.195299	-4.171054	-2.537725
H	-2.345819	-2.179840	-2.619464
C	-4.875990	-4.544802	-0.827125
H	-5.332597	-2.849848	0.448913
C	-4.101309	-5.035458	-1.893551
H	-2.584450	-4.540157	-3.378970
H	-5.591630	-5.209825	-0.314908
H	-4.203198	-6.082786	-2.222553
C	-0.948006	-0.340635	-0.780632
N	-2.100087	-0.499746	-0.616802
P	0.778849	2.365723	-0.125079
C	-0.738496	2.696567	0.880410
O	-0.387455	0.623467	2.115577
C	0.806626	0.722550	2.792131
C	1.064718	1.738679	3.728338
C	2.290818	1.749763	4.411638
C	3.246598	0.745807	4.177124
C	2.988835	-0.257176	3.227692
C	1.777141	-0.272594	2.505726
C	-1.572919	3.815254	0.650466
C	-2.774347	3.983133	1.357902
C	-3.168138	3.027294	2.309063
C	-2.348564	1.918911	2.569772
C	-1.144703	1.764519	1.868854
P	1.483269	-1.334577	1.031612
Pd	0.997845	-0.009154	-0.862864
H	0.307700	2.516807	3.905654
H	2.497518	2.554553	5.134053
H	4.203506	0.751916	4.721241
H	3.750453	-1.025320	3.021620
H	-1.292063	4.551303	-0.118017
H	-3.413891	4.853887	1.146070
H	-4.123757	3.128223	2.845498
H	-2.642336	1.147506	3.294861

C	0.214977	-2.570996	1.522063
C	-0.487495	-3.260387	0.509027
C	-0.049502	-2.861272	2.877827
C	-1.446042	-4.229069	0.846093
H	-0.311546	-3.016161	-0.550017
C	-1.006543	-3.835357	3.210817
H	0.488213	-2.319301	3.672173
C	-1.705475	-4.516984	2.197933
H	-2.018164	-4.728814	0.048683
H	-1.217542	-4.052613	4.269993
H	-2.474827	-5.259286	2.461814
C	3.029372	-2.332812	0.870716
C	4.187167	-1.719675	0.338651
C	3.068668	-3.705713	1.194181
C	5.362323	-2.458440	0.145861
H	4.161921	-0.655153	0.055145
C	4.244366	-4.448518	0.983225
H	2.176584	-4.202608	1.605424
C	5.391635	-3.829544	0.460973
H	6.251171	-1.968106	-0.280110
H	4.258342	-5.522273	1.229437
H	6.307886	-4.415835	0.288067
C	0.517653	3.462753	-1.575658
C	1.393705	4.508680	-1.937225
C	-0.571979	3.142781	-2.424686
C	1.177731	5.227384	-3.128110
H	2.245788	4.765322	-1.287664
C	-0.791343	3.875822	-3.599922
H	-1.260398	2.323594	-2.156852
C	0.086681	4.917392	-3.958330
H	1.866409	6.042598	-3.402793
H	-1.653846	3.626514	-4.238226
H	-0.080924	5.486889	-4.886294
C	2.120375	3.162026	0.861017
C	1.929766	4.387849	1.537926
C	3.353160	2.489375	0.978919
C	2.963949	4.929878	2.317137
H	0.963590	4.912029	1.463555
C	4.385444	3.031406	1.762949
H	3.486778	1.519855	0.473861
C	4.192073	4.251544	2.432575
H	2.808491	5.884330	2.845274
H	5.337826	2.487752	1.864359
H	4.997599	4.672937	3.054940
H	2.596941	0.140928	-1.139649
C	1.141145	0.079966	-3.042289
C	2.537960	0.015178	-2.709220
H	0.729008	1.045325	-3.383085
H	0.630899	-0.815780	-3.431500
C	3.281566	-1.296356	-2.848583
C	4.620478	-1.325230	-3.296741
C	2.667407	-2.526461	-2.510073
C	5.317996	-2.542238	-3.408756
H	5.137149	-0.394173	-3.570744
C	3.360394	-3.737467	-2.620081
H	1.641780	-2.522342	-2.107875
C	4.695168	-3.751936	-3.067037
H	6.362316	-2.536984	-3.759907
H	2.862557	-4.675275	-2.328481
H	5.247633	-4.702213	-3.135329
C	3.341280	1.299780	-2.915604
H	4.256467	1.341721	-2.291864
H	3.645952	1.375821	-3.980617
H	2.723900	2.188590	-2.684264

TS3'-b

Free Energy **=** -3437.321156

Energy = -3438.185224

B	3.672710	0.160444	0.145906
C	3.587901	0.311473	1.775924
C	2.549354	-0.295730	2.523322
C	4.565931	1.028152	2.504714
C	2.475372	-0.179044	3.922057
H	1.765568	-0.870200	2.000695
C	4.509382	1.146135	3.906616
H	5.387475	1.518150	1.956033
C	3.456649	0.547911	4.621920
H	1.643811	-0.653701	4.464547
H	5.286401	1.717130	4.442188
H	3.399280	0.647039	5.718466
C	4.205445	-1.320823	-0.317421
C	4.852766	-2.215438	0.565134
C	4.052393	-1.748847	-1.659658
C	5.326665	-3.471075	0.134541
H	4.987698	-1.921967	1.619685
C	4.506874	-3.002907	-2.102081
H	3.567642	-1.068153	-2.381194
C	5.151501	-3.873145	-1.201582
H	5.828903	-4.143118	0.850422
H	4.367540	-3.302198	-3.154620
H	5.513989	-4.857445	-1.540640
C	4.517616	1.390398	-0.526102
C	3.973134	2.699375	-0.540610
C	5.819924	1.229680	-1.050218
C	4.687438	3.792595	-1.059554
H	2.963438	2.866637	-0.124875
C	6.548933	2.318554	-1.568201
H	6.276656	0.225243	-1.054495
C	5.983630	3.605576	-1.577768
H	4.233718	4.798141	-1.055539
H	7.564541	2.159901	-1.968785
H	6.549580	4.460034	-1.984594
C	1.087483	0.338835	-0.695095
N	2.218779	0.279978	-0.379506
P	-1.469692	-1.522083	0.446961
C	-1.191316	-1.291789	2.287119
O	-1.877667	1.039671	2.192243
C	-3.140873	1.215626	1.682154
C	-4.286462	0.623368	2.234674
C	-5.525518	0.829236	1.608028
C	-5.607618	1.611120	0.442440
C	-4.450698	2.198877	-0.099719
C	-3.196087	2.028252	0.524105
C	-0.706228	-2.338714	3.106577
C	-0.590504	-2.189413	4.498495

C	-0.941279	-0.974660	5.111238
C	-1.391782	0.092116	4.320212
C	-1.518579	-0.072709	2.931523
P	-1.563191	2.395041	-0.263868
Pd	-0.855341	0.314543	-1.157522
H	-4.192773	-0.014799	3.125600
H	-6.427368	0.353903	2.023231
H	-6.575912	1.752202	-0.062178
H	-4.526117	2.765358	-1.039987
H	-0.416776	-3.295318	2.647657
H	-0.211926	-3.028063	5.102968
H	-0.843352	-0.847647	6.200554
H	-1.644156	1.071065	4.753908
C	-0.439163	3.266147	0.928376
C	0.517961	2.508809	1.639639
C	-0.448002	4.671256	1.070960
C	1.450709	3.139787	2.475627
H	0.543343	1.415363	1.542393
C	0.485001	5.300835	1.913799
H	-1.169766	5.288386	0.515323
C	1.437429	4.539258	2.612600
H	2.197205	2.528550	3.004613
H	0.470735	6.398211	2.012879
H	2.178346	5.035982	3.259103
C	-1.885145	3.698183	-1.527793
C	-1.045659	3.701184	-2.664233
C	-2.844442	4.726359	-1.378519
C	-1.172826	4.700240	-3.643118
H	-0.276659	2.917497	-2.763999
C	-2.976971	5.718036	-2.365857
H	-3.483298	4.764276	-0.482691
C	-2.146028	5.705038	-3.500295
H	-0.506662	4.692931	-4.520397
H	-3.730232	6.512515	-2.242186
H	-2.251665	6.485161	-4.270959
C	-0.567313	-3.121828	0.224723
C	-1.182454	-4.390258	0.295866
C	0.838951	-3.044358	0.104311
C	-0.396561	-5.555877	0.292903
H	-2.277882	-4.473827	0.361706
C	1.621316	-4.209577	0.118373
H	1.338513	-2.070633	0.005763
C	1.005149	-5.468275	0.222806
H	-0.888108	-6.540578	0.349102
H	2.715244	-4.119043	0.035714
H	1.617936	-6.383895	0.233207
C	-3.268659	-1.988964	0.473668
C	-3.841469	-2.710645	1.547131
C	-4.100724	-1.574433	-0.585515
C	-5.212545	-3.013422	1.549932
H	-3.215189	-3.024441	2.396661
C	-5.472284	-1.877145	-0.583092
H	-3.674720	-0.975312	-1.403899
C	-6.032176	-2.598318	0.484517
H	-5.645203	-3.571923	2.395432
H	-6.108440	-1.530778	-1.412807
H	-7.109500	-2.828618	0.492776
H	-2.322658	0.362544	-1.789295
C	-1.682847	0.160613	-3.311346
C	-0.471466	-0.588998	-3.310750
H	-1.665737	1.186488	-3.715359
H	-2.642937	-0.356318	-3.477162
C	-0.486190	-2.074960	-3.207793
C	0.728990	-2.802439	-3.206013
C	-1.693521	-2.815906	-3.104954
C	0.739534	-4.201380	-3.106735
H	1.688387	-2.269731	-3.241765
C	-1.682948	-4.212129	-3.015514
H	-2.664363	-2.300084	-3.091035
C	-0.464641	-4.916853	-3.017118
H	1.704609	-4.730239	-3.073204
H	-2.636750	-4.756281	-2.928259
H	-0.455716	-6.013849	-2.926577
C	0.780255	0.071871	-3.867279
H	1.701768	-0.197924	-3.318652
H	0.921099	-0.243886	-4.925186
H	0.699441	1.175439	-3.844168

TS3-c

Free Energy = -3398.027247

Energy = -3398.865764

B	-3.544351	-0.937312	-0.399875
C	-3.919257	-0.733260	1.180366
C	-3.102417	-1.321541	2.175454
C	-5.075675	-0.051740	1.620973
C	-3.422698	-1.250983	3.540893
H	-2.187253	-1.843722	1.865289
C	-5.405047	0.038202	2.988328
H	-5.733905	0.426597	0.876238
C	-4.580956	-0.564941	3.956044
H	-2.758710	-1.724730	4.283152
H	-6.314367	0.579356	3.300345
H	-4.839263	-0.501117	5.026140
C	-4.313886	0.124760	-1.378223
C	-4.015758	1.505656	-1.260414
C	-5.268289	-0.245583	-2.350519
C	-4.621818	2.471414	-2.080809
H	-3.287043	1.828690	-0.498906
C	-5.892393	0.713285	-3.174102
H	-5.525214	-1.311908	-2.471903
C	-5.567797	2.075600	-3.047041
H	-4.356483	3.536096	-1.965264
H	-6.633916	0.393169	-3.925538
H	-6.050858	2.825859	-3.694893
C	-3.704012	-2.509395	-0.847675
C	-2.985416	-3.032325	-1.951347
C	-4.539539	-3.410964	-0.148404
C	-3.075532	-4.383798	-2.328668
H	-2.321483	-2.361645	-2.524446
C	-4.644599	-4.765891	-0.516813
H	-5.110726	-3.046000	0.721418
C	-3.906077	-5.261930	-1.606056
H	-2.494194	-4.757455	-3.188633
H	-5.301711	-5.441601	0.056227
H	-3.977899	-6.324144	-1.892471

C	-0.897992	-0.400409	-0.772151
N	-2.035352	-0.611031	-0.569741
P	0.676779	2.416652	-0.279146
C	-0.806411	2.694613	0.789255
O	-0.255582	0.690902	2.064238
C	0.955720	0.865208	2.693993
C	1.197947	1.911490	3.600752
C	2.446025	1.993784	4.237751
C	3.440541	1.032243	3.986545
C	3.198409	0.000747	3.064116
C	1.963626	-0.086328	2.388427
C	-1.718928	3.753079	0.573285
C	-2.878669	3.881145	1.354984
C	-3.148263	2.947975	2.370287
C	-2.249065	1.899343	2.615409
C	-1.090787	1.780758	1.835761
P	1.663492	-1.196856	0.950896
Pd	1.018509	0.051847	-0.956800
H	0.411968	2.657110	3.791295
H	2.639447	2.821242	4.937867
H	4.414538	1.094803	4.495631
H	3.987932	-0.733705	2.841109
H	-1.532425	4.470596	-0.240511
H	-3.583012	4.702930	1.153303
H	-4.068685	3.019731	2.969249
H	-2.445744	1.146200	3.390485
C	0.467088	-2.469756	1.527362
C	-0.234479	-3.224754	0.561745
C	0.251089	-2.717879	2.899893
C	-1.146595	-4.213730	0.961943
H	-0.097423	-3.014202	-0.510358
C	-0.657867	-3.714331	3.296500
H	0.787500	-2.124866	3.657802
C	-1.358888	-4.458572	2.330348
H	-1.721535	-4.763215	0.200092
H	-0.831721	-3.898085	4.368643
H	-2.093791	-5.216568	2.643097
C	3.244580	-2.132833	0.766527
C	4.343494	-1.497709	0.144127
C	3.369701	-3.477458	1.176025
C	5.548543	-2.186725	-0.050606
H	4.248055	-0.457699	-0.208111
C	4.574852	-4.170808	0.964352
H	2.522258	-3.989212	1.657284
C	5.665207	-3.529154	0.354119
H	6.391933	-1.681434	-0.545732
H	4.657731	-5.223092	1.280064
H	6.605034	-4.077524	0.182807
C	0.305851	3.440926	-1.757191
C	1.137445	4.487939	-2.207971
C	-0.820177	3.062549	-2.531396
C	0.839207	5.154774	-3.410930
H	2.016424	4.790150	-1.616477
C	-1.121748	3.745015	-3.718889
H	-1.471551	2.238407	-2.194808
C	-0.289940	4.790943	-4.164817
H	1.493084	5.972253	-3.755259
H	-2.012295	3.452174	-4.297533
H	-0.522906	5.321360	-5.101863
C	2.005098	3.313598	0.635210
C	1.778953	4.570256	1.241271
C	3.258948	2.688010	0.784271
C	2.801012	5.190465	1.976885
H	0.795027	5.057336	1.147340
C	4.279142	3.308796	1.524240
H	3.417295	1.689889	0.346195
C	4.052056	4.560779	2.120061
H	2.618316	6.169025	2.449345
H	5.248314	2.801397	1.650396
H	4.848239	5.044830	2.707913
H	2.581858	0.343281	-1.323314
C	1.002686	0.038447	-3.147277
C	2.401979	-0.021960	-2.859346
H	2.966798	0.907525	-3.064348
H	0.570865	0.988202	-3.504845
H	0.475079	-0.876624	-3.463012
C	3.225189	-1.266769	-2.976501
C	4.553703	-1.170899	-3.443789
C	2.727955	-2.536224	-2.601643
C	5.360949	-2.316892	-3.549659
H	4.959335	-0.186105	-3.729121
C	3.532696	-3.678001	-2.703409
H	1.711537	-2.615036	-2.184622
C	4.854757	-3.572714	-3.176216
H	6.395783	-2.224364	-3.916221
H	3.134960	-4.654189	-2.385308
H	5.492352	-4.468554	-3.238877

TS3'-c

Free Energy **=** -3398.016114

Energy = -3398.855189

B	3.699929	-0.001282	-0.041339
C	3.653149	0.148560	1.591736
C	2.582146	-0.367978	2.360859
C	4.703918	0.774864	2.303305
C	2.546271	-0.250976	3.761039
H	1.737110	-0.867474	1.858308
C	4.686218	0.891925	3.706297
H	5.554002	1.194971	1.740374
C	3.600692	0.384767	4.442492
H	1.686674	-0.653131	4.318174
H	5.520929	1.391319	4.226381
H	3.574629	0.484122	5.540193
C	4.128831	-1.512821	-0.511883
C	4.860425	-2.386520	0.325477
C	3.814210	-1.987138	-1.809474
C	5.262458	-3.666251	-0.106322
H	5.119445	-2.056679	1.345672
C	4.197168	-3.265765	-2.250393
H	3.252412	-1.329028	-2.495069
C	4.928775	-4.113900	-1.397008
H	5.833227	-4.320936	0.573421
H	3.929006	-3.603613	-3.265717
H	5.234246	-5.117303	-1.736217
C	4.629625	1.165758	-0.712925

C	4.183233	2.511166	-0.725952
C	5.920558	0.910621	-1.227444
C	4.982609	3.550978	-1.230372
H	3.183991	2.750327	-0.320475
C	6.734127	1.944997	-1.730543
H	6.300386	-0.125381	-1.233469
C	6.266780	3.270846	-1.736046
H	4.605682	4.587740	-1.224751
H	7.738859	1.713160	-2.122677
H	6.899547	4.083154	-2.130605
C	1.125113	0.326132	-0.865488
N	2.253079	0.218115	-0.551470
P	-1.491242	-1.401667	0.471150
C	-1.177925	-1.172522	2.304808
O	-1.732179	1.187540	2.171100
C	-2.995448	1.414368	1.682141
C	-4.157581	0.901258	2.279068
C	-5.398886	1.156132	1.676247
C	-5.468941	1.907537	0.489863
C	-4.296569	2.416306	-0.096311
C	-3.038001	2.196539	0.503488
C	-0.747346	-2.234734	3.134595
C	-0.604777	-2.069090	4.522280
C	-0.869511	-0.823991	5.117668
C	-1.264580	0.256011	4.314565
C	-1.421713	0.073883	2.931460
P	-1.412958	2.473109	-0.335436
Pd	-0.841743	0.368473	-1.249792
H	-4.075501	0.284042	3.185709
H	-6.314098	0.741855	2.126028
H	-6.440654	2.085206	0.003784
H	-4.364001	2.960161	-1.050538
H	-0.521588	-3.214169	2.687696
H	-0.271428	-2.919209	5.137312
H	-0.747922	-0.685368	6.203172
H	-1.450854	1.255525	4.734474
C	-0.211304	3.298723	0.811136
C	0.725409	2.500569	1.504180
C	-0.144566	4.703912	0.936467
C	1.713272	3.091197	2.305570
H	0.691849	1.406847	1.417751
C	0.842812	5.293172	1.745834
H	-0.847719	5.351805	0.392294
C	1.774754	4.490839	2.426387
H	2.442830	2.448296	2.820875
H	0.887520	6.390780	1.832056
H	2.558210	4.955718	3.045822
C	-1.710707	3.774569	-1.606595
C	-0.918919	3.723255	-2.775641
C	-2.606475	4.854169	-1.426899
C	-1.032366	4.722432	-3.756460
H	-0.197007	2.899065	-2.901376
C	-2.724345	5.846074	-2.415664
H	-3.206947	4.931289	-0.507211
C	-1.942068	5.780268	-3.582396
H	-0.404703	4.673571	-4.660356
H	-3.427625	6.681150	-2.267962
H	-2.035601	6.560618	-4.354396
C	-0.655137	-3.036108	0.247938
C	-1.320242	-4.279009	0.285728
C	0.756025	-3.012482	0.151014
C	-0.578994	-5.474423	0.272690
H	-2.418835	-4.321638	0.330883
C	1.492716	-4.205847	0.154834
H	1.294206	-2.057964	0.075073
C	0.825285	-5.441331	0.226328
H	-1.109722	-6.439729	0.299265
H	2.590419	-4.157671	0.090217
H	1.401291	-6.380503	0.227853
C	-3.307710	-1.788324	0.528450
C	-3.885522	-2.524792	1.589140
C	-4.146772	-1.293141	-0.489340
C	-5.267911	-2.769007	1.615647
H	-3.252955	-2.898061	2.409526
C	-5.529668	-1.537221	-0.463546
H	-3.714408	-0.672481	-1.288933
C	-6.094068	-2.278230	0.587819
H	-5.704061	-3.341818	2.449709
H	-6.170246	-1.128125	-1.260636
H	-7.179621	-2.464432	0.614039
H	-2.319273	0.495317	-1.861376
C	-1.670371	0.157795	-3.368061
C	-0.632481	-0.799896	-3.202923
H	0.388877	-0.486610	-3.477098
H	-1.440520	1.131945	-3.828421
H	-2.697339	-0.192385	-3.572082
C	-0.841037	-2.255096	-3.100859
C	0.290274	-3.105760	-3.055618
C	-2.128432	-2.847004	-3.053210
C	0.143005	-4.497762	-3.002318
H	1.297234	-2.661168	-3.034634
C	-2.274409	-4.238979	-2.996937
H	-3.029565	-2.215631	-3.063763
C	-1.140022	-5.071779	-2.979633
H	1.038610	-5.135809	-2.952091
H	-3.283670	-4.678768	-2.958837
H	-1.256258	-6.165460	-2.926172

TS3-d

Free Energy **=** -3437.32062

Energy = -3438.183401

B	4.066157	0.303481	-0.611889
C	4.390228	0.094282	0.980215
C	3.620238	-0.770557	1.795520
C	5.480408	0.750707	1.599116
C	3.910019	-0.961719	3.158297
H	2.757196	-1.305064	1.362245
C	5.784138	0.567274	2.961059
H	6.099990	1.436919	0.998044
C	4.994389	-0.288238	3.750048
H	3.280901	-1.635728	3.758854
H	6.638012	1.101328	3.410895
H	5.221535	-0.430260	4.819534
C	4.584709	-0.949689	-1.535783
C	5.405975	-1.987844	-1.041170

C	4.224017	-1.015460	-2.905346
C	5.856648	-3.035630	-1.869606
H	5.703954	-1.975849	0.020861
C	4.665786	-2.052827	-3.743649
H	3.580582	-0.222394	-3.324617
C	5.490830	-3.070809	-3.226769
H	6.498465	-3.829351	-1.451608
H	4.366141	-2.071957	-4.804945
H	5.841996	-3.888065	-3.878114
C	4.603818	1.759948	-1.136902
C	3.954998	2.948710	-0.717711
C	5.749752	1.906252	-1.950888
C	4.418610	4.219437	-1.097809
H	3.066497	2.875044	-0.066376
C	6.227925	3.174869	-2.334900
H	6.281482	1.003171	-2.295983
C	5.561548	4.338172	-1.911921
H	3.888630	5.123729	-0.753736
H	7.125830	3.255057	-2.970837
H	5.930468	5.332663	-2.213340
C	1.353907	0.353731	-0.854715
N	2.524962	0.331113	-0.762739
P	-0.863071	-1.967142	0.276886
C	-0.072761	-2.280380	1.929971
O	-0.779124	-0.083556	2.707392
C	-2.139889	0.052334	2.555213
C	-3.058831	-0.758343	3.242959
C	-4.431999	-0.569452	3.028894
C	-4.875864	0.408816	2.122442
C	-3.947264	1.211526	1.439597
C	-2.560471	1.068715	1.663899
C	0.638707	-3.464902	2.228631
C	1.183876	-3.686057	3.504091
C	1.034539	-2.718015	4.512251
C	0.352769	-1.522746	4.236001
C	-0.194528	-1.314359	2.960877
P	-1.264885	1.867042	0.606464
Pd	-0.634047	0.275307	-1.007562
H	-2.686573	-1.543888	3.917175
H	-5.155845	-1.213311	3.551608
H	-5.950106	0.532869	1.917344
H	-4.313242	1.927750	0.690872
H	0.772043	-4.225153	1.443589
H	1.733985	-4.618000	3.706671
H	1.465401	-2.883290	5.512029
H	0.243040	-0.729084	4.989567
C	0.060032	2.615778	1.668717
C	1.203262	1.848546	1.985631
C	0.000818	3.964510	2.085023
C	2.264144	2.412590	2.709278
H	1.277354	0.803511	1.660420
C	1.065444	4.526524	2.811713
H	-0.864966	4.594151	1.831569
C	2.197966	3.754907	3.122837
H	3.150795	1.798699	2.929211
H	1.009308	5.581529	3.124710
H	3.037870	4.201814	3.678108
C	-2.090232	3.339530	-0.139623
C	-1.711040	3.699803	-1.451464
C	-3.039903	4.132522	0.544760
C	-2.295045	4.810251	-2.083001
H	-0.952726	3.094936	-1.976334
C	-3.630954	5.236183	-0.094086
H	-3.323526	3.890249	1.580488
C	-3.266703	5.572198	-1.410256
H	-1.992116	5.077792	-3.107553
H	-4.379153	5.840030	0.443765
H	-3.735103	6.435424	-1.909210
C	-0.023356	-3.194698	-0.808184
C	-0.740872	-4.131605	-1.583780
C	1.373699	-3.061869	-1.002580
C	-0.067814	-4.922861	-2.533997
H	-1.828190	-4.244615	-1.447290
C	2.041275	-3.860452	-1.941447
H	1.951397	-2.323805	-0.426285
C	1.319842	-4.790885	-2.713981
H	-0.636727	-5.651027	-3.134677
H	3.127267	-3.739235	-2.075952
H	1.843112	-5.410155	-3.459841
C	-2.546475	-2.684927	0.555857
C	-2.741740	-3.893978	1.263301
C	-3.666022	-1.983371	0.069221
C	-4.038006	-4.389260	1.471271
H	-1.875628	-4.447568	1.658610
C	-4.963995	-2.482076	0.276417
H	-3.530186	-1.013909	-0.433381
C	-5.152631	-3.684073	0.976563
H	-4.180820	-5.330844	2.025593
H	-5.825436	-1.907570	-0.095797
H	-6.170072	-4.071066	1.147386
H	-2.175326	0.412401	-1.445637
C	-0.521422	-0.553695	-3.025482
C	-1.774608	0.124193	-3.020748
H	-1.775066	1.157011	-3.415602
H	-0.497457	-1.657549	-3.008695
H	0.354476	-0.064726	-3.479650
C	-3.085094	-0.623468	-3.215577
H	-3.189262	-0.794719	-4.312614
H	-3.001099	-1.636081	-2.763790
C	-4.343827	0.058531	-2.702727
C	-5.544552	-0.681695	-2.612438
C	-4.362801	1.408339	-2.290521
C	-6.719208	-0.097234	-2.112963
H	-5.549089	-1.739757	-2.922149
C	-5.537054	1.997280	-1.786558
H	-3.456674	2.026666	-2.346971
C	-6.718835	1.245732	-1.689228
H	-7.641645	-0.696407	-2.045887
H	-5.513097	3.051938	-1.467822
H	-7.638733	1.702284	-1.290551

TS3'-d

Free Energy = -3437.316494

Energy = -3438.181895

B	3.964190	0.040293	-0.589469

C	4.237624	1.274808	0.448177	H	2.208687	0.751259	3.680425
C	3.209471	1.946078	1.147928	C	-0.162567	3.271801	0.051486
C	5.566001	1.697910	0.706834	C	0.733743	3.361735	-1.035014
C	3.486722	2.961589	2.082427	C	-0.037953	4.179643	1.127114
H	2.158754	1.678987	0.960332	C	1.733978	4.346463	-1.049895
C	5.857093	2.711462	1.636945	H	0.671165	2.637403	-1.861358
H	6.395848	1.221487	0.156718	C	0.960619	5.167703	1.103962
C	4.814143	3.346901	2.337603	H	-0.719909	4.111374	1.989782
H	2.652670	3.457357	2.605335	C	1.849339	5.251547	0.018404
H	6.903744	3.012199	1.813754	H	2.445107	4.388405	-1.889302
H	5.036545	4.143081	3.067562	H	1.055365	5.866220	1.950601
C	4.345186	-1.430208	0.041660	H	2.648717	6.008727	0.015750
C	5.183405	-1.610155	1.165070	C	-2.950277	2.835060	-0.693918
C	3.854019	-2.607822	-0.574739	C	-3.927552	2.048310	-1.343596
C	5.522464	-2.890847	1.643998	C	-3.130813	4.232959	-0.599737
H	5.576934	-0.724354	1.690261	C	-5.076528	2.654770	-1.879356
C	4.158078	-3.892124	-0.092259	H	-3.783586	0.957856	-1.436589
H	3.218537	-2.511161	-1.471972	C	-4.278223	4.834026	-1.144171
C	5.003952	-4.040478	1.023283	H	-2.369981	4.855799	-0.103461
H	6.183782	-2.990344	2.521412	C	-5.253419	4.046091	-1.781838
H	3.741165	-4.782812	-0.592166	H	-5.829656	2.029770	-2.382186
H	5.256494	-5.044193	1.403392	H	-4.408801	5.925655	-1.071813
C	4.755130	0.321555	-2.001121	H	-6.151207	4.519619	-2.210537
C	4.272966	1.286256	-2.919607	C	-0.804428	-3.319328	-0.094656
C	5.971276	-0.321109	-2.327667	C	-1.796669	-4.306128	0.078734
C	4.962070	1.593842	-4.105122	C	0.288531	-3.574396	-0.956847
H	3.329122	1.813075	-2.691717	C	-1.700369	-5.530187	-0.609982
C	6.677135	-0.016757	-3.508171	H	-2.651734	-4.123005	0.747411
H	6.375094	-1.084565	-1.640877	C	0.385651	-4.800380	-1.629692
C	6.173537	0.941309	-4.404932	H	1.061557	-2.803275	-1.097659
H	4.557099	2.349037	-4.800352	C	-0.613142	-5.779839	-1.463449
H	7.624208	-0.536521	-3.732012	H	-2.485156	-6.291551	-0.476088
H	6.720162	1.178878	-5.332608	H	1.244780	-4.989186	-2.292784
C	1.305367	-0.076545	-1.178381	H	-0.541117	-6.738936	-2.000446
N	2.452810	-0.008513	-0.920895	C	-2.334179	-1.738997	1.820701
P	-0.920227	-1.631568	0.634335	C	-2.245543	-2.558574	2.969462
C	0.528190	-1.578677	1.786368	C	-3.503764	-0.989894	1.590235
O	0.160500	0.798763	2.060208	C	-3.325016	-2.637414	3.862659
C	-1.049387	1.104927	2.639544	H	-1.325173	-3.130810	3.168066
C	-1.389944	0.747344	3.953371	C	-4.580266	-1.067156	2.489674
C	-2.631600	1.155802	4.467554	H	-3.563416	-0.331751	0.710799
C	-3.515389	1.919141	3.683553	C	-4.494825	-1.892190	3.623600
C	-3.176689	2.245264	2.359625	H	-3.249612	-3.278884	4.755151
C	-1.946907	1.825773	1.815413	H	-5.482172	-0.461726	2.309437
C	1.326322	-2.705881	2.079053	H	-5.336910	-1.946276	4.331893
C	2.419382	-2.602706	2.953075	H	-0.864502	1.104948	-2.220643
C	2.743023	-1.368739	3.539078	C	-1.362975	0.039334	-3.455289
C	1.963641	-0.235035	3.262850	C	-1.225291	-1.305227	-3.106613
C	0.865527	-0.350177	2.400203	H	-0.221814	-1.756668	-3.190646
P	-1.485521	1.981105	0.041230	H	-0.524921	0.545321	-3.963982
Pd	-0.824941	0.045492	-1.039816	H	-2.363171	0.476061	-3.618539
H	-0.688787	0.149280	4.554111	C	-2.356639	-2.311968	-3.043003
H	-2.909116	0.871269	5.494497	H	-2.358262	-2.828110	-4.033071
H	-4.483803	2.241622	4.095939	H	-2.103057	-3.104604	-2.311558
H	-3.885646	2.805959	1.730971	C	-3.736809	-1.763499	-2.761989
H	1.104756	-3.673331	1.605009	C	-4.302173	-1.891920	-1.477552
H	3.044013	-3.487241	3.143007	C	-4.485093	-1.104260	-3.762875
H	3.621515	-1.279001	4.195817	C	-5.576176	-1.373443	-1.191154

H	-3.737847	-2.423136	-0.697351	H	-5.994074	-1.488376	-0.178464
C	-5.761118	-0.585641	-3.482786	H	-6.332413	-0.079948	-4.277757
H	-4.067433	-1.010424	-4.778972	H	-7.311925	-0.314458	-1.973970
C	-6.310483	-0.717307	-2.193989				