

Tryptophan Lyase (NosL): Mechanistic Insights into Amine Dehydrogenation and Carboxyl Fragment Migration by QM/MM calculations

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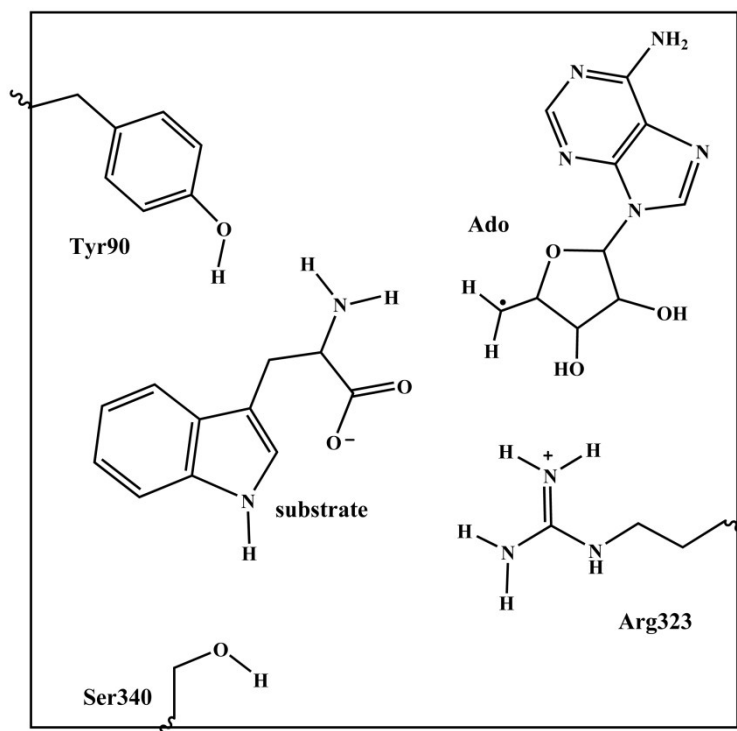


Figure S1. QM region for QM/MM calculations.

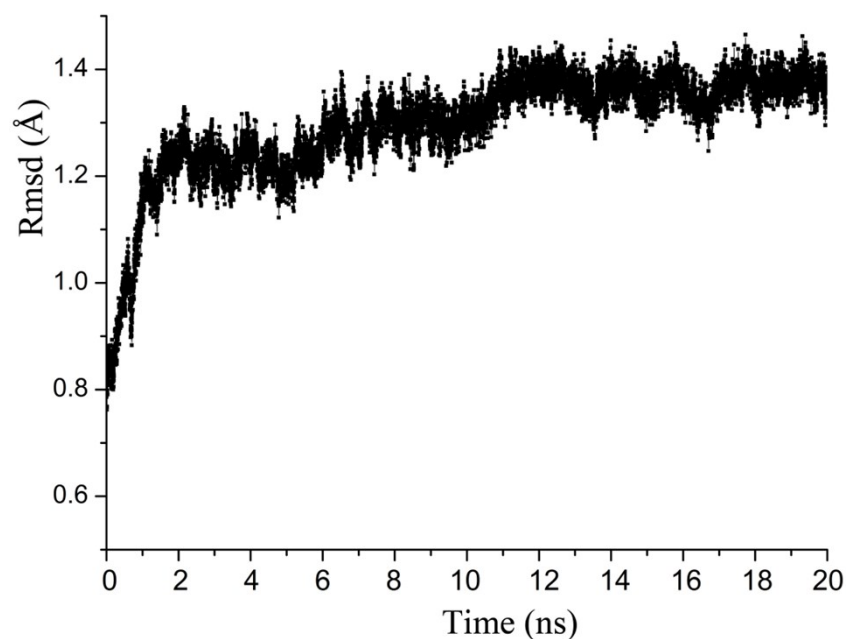


Figure S2. RMSDs of NosL from 20ns of MD simulation.

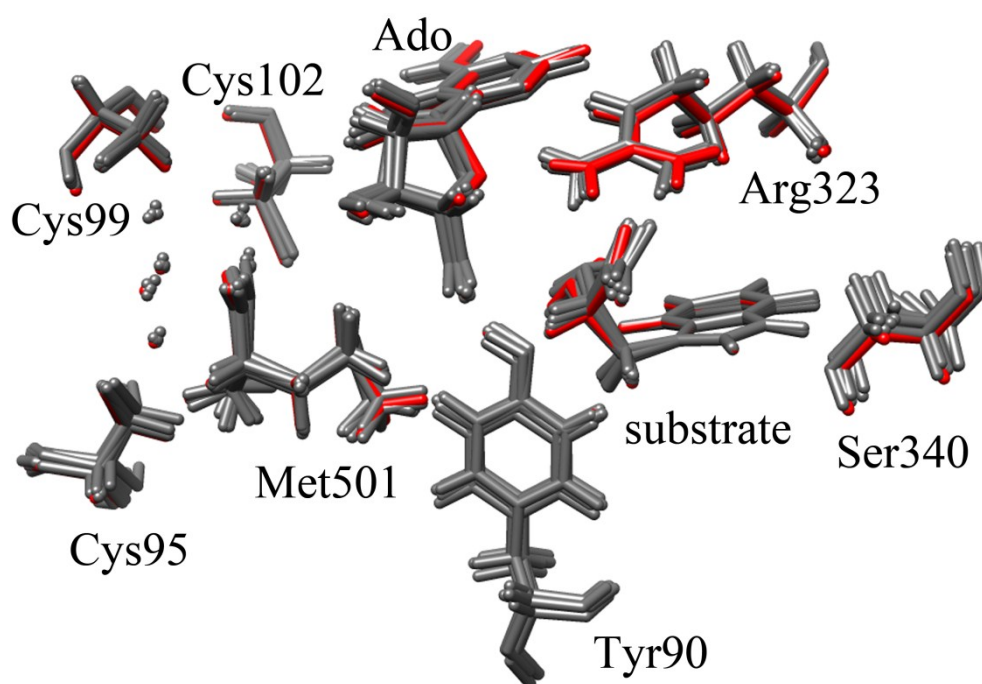


Figure S3. Superposition of 11 optimized QM/MM structures that were picked up from 10 to 20 ns of MD trajectory. The RMSDs of these structures relative to the average one are 0.37, 0.45, 0.43, 0.45, 0.39, 0.45, 0.43, 0.49, 0.41, 0.40 and 0.35.

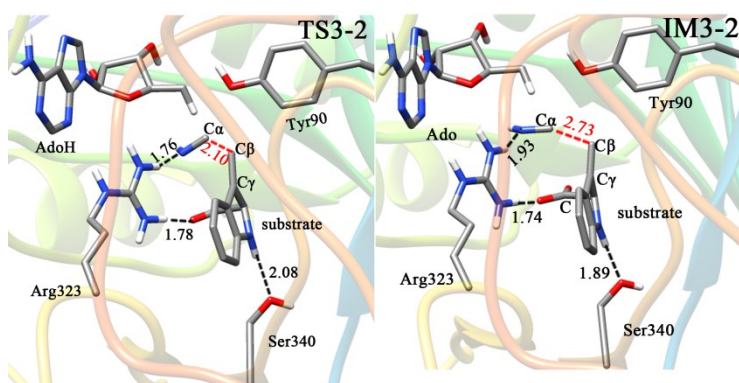


Figure S4. Optimized structures of transition state (TS3-2) and intermediate (IM3-2) in path2.

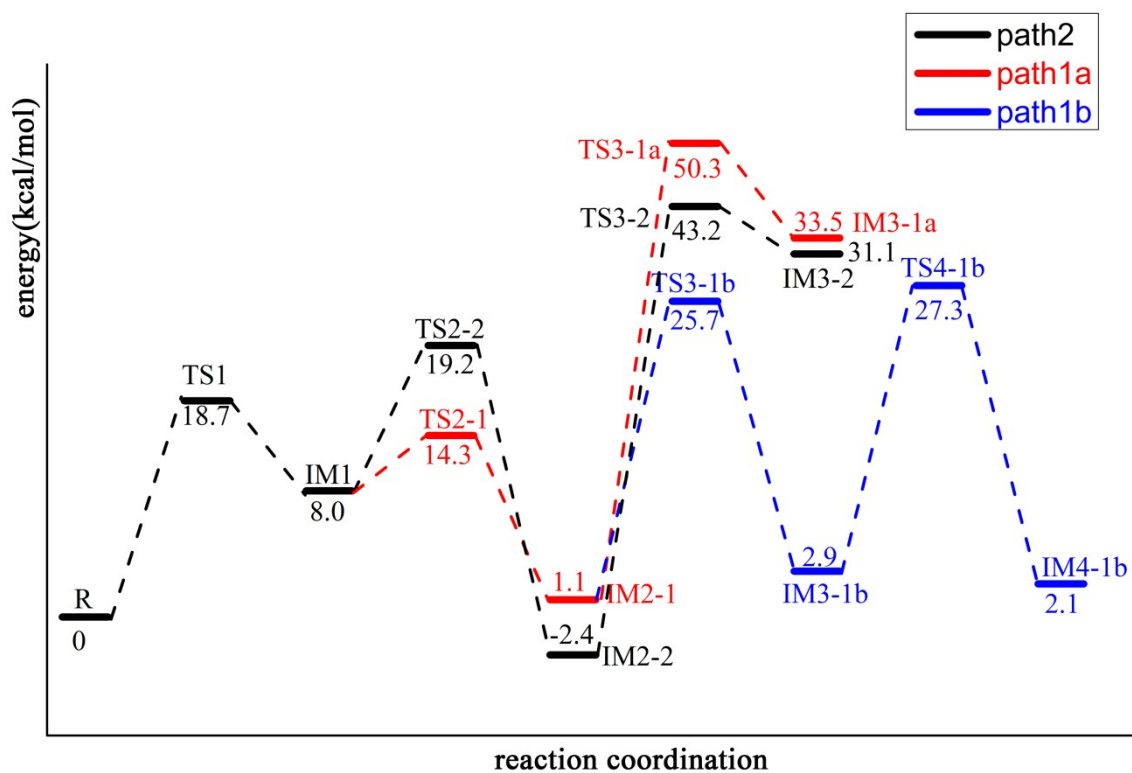


Figure S5. Energy profiles for NosL with M06 functional.

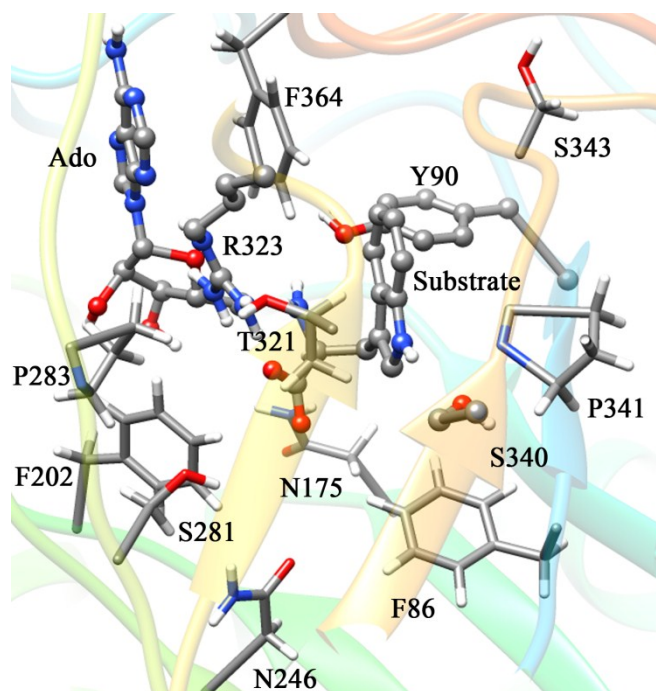


Figure S6. Surrounding residues around the substrate. QM atoms are shown in ball-and-stick model.

Absolute QM/MM single-point energies (E , a.u.) with b3lyp/6-311++G(2d,2p) and the dispersion correction (ΔE , a.u.) as well as Cartesian coordinates of QM regions:

R				H	-1.695	-2.254	-9.564
E=-2454.536567		$\Delta E=-0.196184$		H	-1.746	-3.265	-8.116
C	-12.229	1.370	-4.472	C	-0.104	-1.840	-8.158
H	-12.627	0.626	-5.173	H	0.557	-2.410	-7.495
H	-12.696	2.331	-4.716	H	0.548	-1.369	-8.902
C	-10.726	1.532	-4.642	N	-0.730	-0.765	-7.385
C	-9.804	0.483	-4.475	H	-0.748	0.166	-7.790
H	-10.144	-0.498	-4.157	C	-0.995	-0.842	-6.060
C	-8.447	0.660	-4.717	N	-0.934	-2.002	-5.405
H	-7.746	-0.159	-4.589	H	-1.137	-1.973	-4.401
C	-7.965	1.901	-5.155	H	-0.805	-2.903	-5.858
O	-6.632	2.010	-5.403	N	-1.328	0.256	-5.372
H	-6.442	2.870	-5.839	H	-1.536	0.133	-4.371
C	-10.220	2.771	-5.051	H	-1.363	1.181	-5.788
H	-10.900	3.611	-5.182	C	-3.029	-7.726	-1.759
C	-8.863	2.961	-5.313	H	-2.487	-7.696	-0.805
H	-8.499	3.930	-5.642	H	-2.420	-7.230	-2.513
C	-0.238	-3.877	-9.589	O	-4.270	-7.049	-1.676
H	0.471	-4.338	-8.890	H	-4.796	-7.452	-0.956
H	0.366	-3.369	-10.352	N	-3.574	1.072	-2.716
C	-1.072	-2.816	-8.855	H	-3.279	1.554	-1.860

H	-4.447	1.498	-3.014
C	-3.798	-0.358	-2.437
H	-4.513	-0.533	-1.617
C	-4.339	-1.007	-3.721
H	-3.716	-0.663	-4.555
H	-5.340	-0.584	-3.909
C	-4.400	-2.509	-3.738
C	-4.220	-3.408	-2.711
H	-3.988	-3.216	-1.673
N	-4.315	-4.703	-3.178
H	-4.314	-5.540	-2.587
C	-4.573	-4.672	-4.527
C	-4.627	-3.302	-4.919
C	-4.863	-2.995	-6.270
H	-4.927	-1.961	-6.598
C	-5.026	-4.033	-7.181
H	-5.184	-3.802	-8.231
C	-4.767	-5.717	-5.441
H	-4.738	-6.748	-5.109
C	-4.985	-5.384	-6.774
H	-5.127	-6.173	-7.506
C	-2.448	-0.954	-1.986
O	-1.507	-1.004	-2.839
O	-2.356	-1.338	-0.789
N	-0.350	2.392	-8.922
C	-0.286	1.940	-10.175
H	0.061	0.915	-10.300
N	-0.572	2.589	-11.315
C	-1.015	3.862	-11.265
N	-1.344	4.474	-12.425
H	-1.091	3.996	-13.285
H	-1.540	5.468	-12.441
C	-1.120	4.466	-9.991
N	-1.489	5.735	-9.584
C	-0.751	3.675	-8.892
N	-0.880	4.493	-7.790
C	-1.330	5.706	-8.282
H	-1.507	6.547	-7.626
C	-0.597	4.083	-6.408
H	0.331	3.510	-6.424
C	-0.485	5.265	-5.426
H	-0.210	6.192	-5.940
O	0.458	4.938	-4.442
H	0.900	5.783	-4.160

C	-1.917	5.321	-4.836
H	-2.582	5.773	-5.592
O	-2.085	6.060	-3.672
H	-1.812	5.529	-2.888
C	-2.246	3.806	-4.739
H	-1.697	3.417	-3.866
C	-3.672	3.450	-4.661
H	-4.123	2.782	-5.383
H	-4.218	3.693	-3.758
O	-1.665	3.254	-5.949

TS1

E=-2454.513978 $\Delta E=-0.199068$

C	-12.206	1.374	-4.448
H	-12.629	0.653	-5.159
H	-12.642	2.353	-4.681
C	-10.698	1.485	-4.620
C	-9.807	0.412	-4.441
H	-10.169	-0.551	-4.096
C	-8.448	0.538	-4.707
H	-7.773	-0.302	-4.572
C	-7.933	1.749	-5.188
O	-6.608	1.793	-5.487
H	-6.384	2.653	-5.907
C	-10.155	2.699	-5.060
H	-10.809	3.558	-5.197
C	-8.797	2.837	-5.349
H	-8.407	3.787	-5.706
C	-0.217	-3.904	-9.619
H	0.484	-4.370	-8.916
H	0.397	-3.407	-10.382
C	-1.035	-2.826	-8.895
H	-1.650	-2.261	-9.608
H	-1.712	-3.256	-8.149
C	-0.045	-1.861	-8.213
H	0.609	-2.436	-7.548
H	0.611	-1.413	-8.968
N	-0.646	-0.762	-7.457
H	-0.601	0.171	-7.857
C	-0.903	-0.806	-6.128
N	-0.900	-1.950	-5.450
H	-1.115	-1.898	-4.442
H	-0.785	-2.858	-5.892
N	-1.157	0.337	-5.478

H	-1.464	0.336	-4.499	N	-0.975	4.434	-7.695
H	-1.261	1.220	-5.965	C	-1.438	5.638	-8.196
C	-3.045	-7.591	-1.818	H	-1.659	6.469	-7.541
H	-2.491	-7.529	-0.873	C	-0.705	4.051	-6.307
H	-2.457	-7.105	-2.594	H	0.222	3.473	-6.306
O	-4.298	-6.929	-1.734	C	-0.581	5.252	-5.343
H	-4.798	-7.330	-0.994	H	-0.388	6.187	-5.879
N	-2.739	1.087	-3.027	O	0.438	4.979	-4.422
H	-2.549	1.609	-2.160	H	0.867	5.842	-4.176
H	-3.323	1.958	-3.689	C	-1.976	5.248	-4.661
C	-3.466	-0.124	-2.634	H	-2.712	5.636	-5.390
H	-4.200	0.049	-1.836	O	-2.101	6.016	-3.511
C	-4.143	-0.791	-3.846	H	-1.816	5.501	-2.721
H	-3.510	-0.607	-4.722	C	-2.197	3.726	-4.526
H	-5.079	-0.250	-4.049	H	-1.475	3.373	-3.773
C	-4.369	-2.278	-3.745	C	-3.568	3.228	-4.187
C	-4.261	-3.101	-2.644	H	-4.254	3.122	-5.028
H	-4.036	-2.847	-1.619	H	-4.001	3.751	-3.334
N	-4.411	-4.421	-3.008	O	-1.783	3.238	-5.833
H	-4.363	-5.231	-2.386				
C	-4.623	-4.487	-4.364	IM1			
C	-4.618	-3.152	-4.864	E=-5454.532784	$\Delta E=-0.194669$		
C	-4.827	-2.952	-6.241	C	-12.228	1.402	-4.484
H	-4.861	-1.946	-6.651	H	-12.625	0.656	-5.183
C	-5.010	-4.056	-7.068	H	-12.701	2.361	-4.730
H	-5.153	-3.909	-8.136	C	-10.727	1.573	-4.662
C	-4.822	-5.599	-5.193	C	-9.796	0.531	-4.504
H	-4.829	-6.600	-4.777	H	-10.126	-0.451	-4.177
C	-5.005	-5.370	-6.553	C	-8.443	0.714	-4.768
H	-5.146	-6.212	-7.224	H	-7.737	-0.103	-4.648
C	-2.316	-0.989	-2.014	C	-7.975	1.954	-5.221
O	-1.409	-1.368	-2.801	O	-6.649	2.067	-5.508
O	-2.353	-1.191	-0.772	H	-6.471	2.941	-5.919
N	-0.361	2.350	-8.825	C	-10.232	2.815	-5.082
C	-0.253	1.907	-10.079	H	-10.919	3.650	-5.207
H	0.125	0.893	-10.201	C	-8.880	3.011	-5.364
N	-0.532	2.552	-11.221	H	-8.525	3.980	-5.703
C	-1.008	3.813	-11.175	C	-0.172	-3.902	-9.664
N	-1.337	4.420	-12.338	H	0.525	-4.358	-8.951
H	-1.066	3.951	-13.196	H	0.444	-3.409	-10.428
H	-1.551	5.410	-12.354	C	-1.007	-2.825	-8.959
C	-1.150	4.410	-9.902	H	-1.601	-2.258	-9.688
N	-1.560	5.669	-9.502	H	-1.704	-3.257	-8.232
C	-0.794	3.622	-8.796	C	-0.044	-1.859	-8.244

H	0.561	-2.424	-7.525
H	0.662	-1.436	-8.968
N	-0.685	-0.740	-7.559
H	-0.651	0.174	-7.998
C	-1.088	-0.744	-6.265
N	-1.118	-1.860	-5.541
H	-1.359	-1.792	-4.535
H	-0.914	-2.771	-5.937
N	-1.469	0.408	-5.704
H	-1.945	0.423	-4.779
H	-1.460	1.272	-6.229
C	-2.910	-7.650	-1.661
H	-2.375	-7.662	-0.703
H	-2.280	-7.150	-2.394
O	-4.132	-6.942	-1.564
H	-4.688	-7.359	-0.875
N	-2.991	0.722	-3.331
H	-3.418	1.636	-3.160
H	-4.029	2.644	-4.772
C	-3.433	-0.148	-2.293
H	-3.697	0.411	-1.388
C	-4.768	-0.921	-2.746
H	-5.252	-0.329	-3.530
H	-5.432	-0.871	-1.876
C	-4.621	-2.353	-3.163
C	-4.362	-3.393	-2.292
H	-4.148	-3.343	-1.235
N	-4.341	-4.590	-2.953
H	-4.259	-5.500	-2.486
C	-4.596	-4.369	-4.284
C	-4.767	-2.961	-4.464
C	-5.045	-2.491	-5.761
H	-5.192	-1.428	-5.937
C	-5.138	-3.401	-6.811
H	-5.325	-3.033	-7.817
C	-4.721	-5.290	-5.334
H	-4.613	-6.356	-5.151
C	-4.983	-4.790	-6.606
H	-5.070	-5.481	-7.441
C	-2.320	-1.148	-1.909
O	-1.565	-1.580	-2.814
O	-2.283	-1.461	-0.687
N	-0.407	2.454	-8.931
C	-0.350	1.988	-10.180

H	-0.029	0.953	-10.293
N	-0.618	2.628	-11.328
C	-1.030	3.912	-11.292
N	-1.353	4.517	-12.457
H	-1.117	4.022	-13.312
H	-1.538	5.513	-12.484
C	-1.112	4.535	-10.027
N	-1.439	5.822	-9.640
C	-0.768	3.750	-8.917
N	-0.866	4.592	-7.828
C	-1.276	5.811	-8.337
H	-1.439	6.664	-7.692
C	-0.714	4.179	-6.435
H	0.137	3.495	-6.388
C	-0.508	5.345	-5.441
H	-0.232	6.271	-5.958
O	0.479	4.975	-4.517
H	0.911	5.814	-4.200
C	-1.909	5.447	-4.780
H	-2.585	5.946	-5.499
O	-1.984	6.171	-3.594
H	-1.765	5.594	-2.827
C	-2.308	3.964	-4.732
H	-1.696	3.455	-3.976
C	-3.776	3.674	-4.518
H	-4.404	4.327	-5.130
H	-4.033	3.860	-3.470
O	-1.916	3.498	-6.050

TS2-1

E=-2454.520222 $\Delta E=-0.199073$

C	-12.157	1.339	-4.448
H	-12.592	0.632	-5.165
H	-12.556	2.331	-4.688
C	-10.642	1.397	-4.600
C	-9.802	0.277	-4.466
H	-10.210	-0.680	-4.161
C	-8.438	0.349	-4.724
H	-7.810	-0.533	-4.637
C	-7.863	1.556	-5.140
O	-6.529	1.557	-5.420
H	-6.272	2.400	-5.857
C	-10.038	2.603	-4.978
H	-10.650	3.498	-5.079

C	-8.671	2.692	-5.249	C	-4.865	-5.336	-5.760
H	-8.233	3.638	-5.554	H	-4.676	-6.404	-5.794
C	-0.056	-3.883	-9.728	C	-5.236	-4.620	-6.897
H	0.602	-4.357	-8.990	H	-5.320	-5.149	-7.842
H	0.600	-3.422	-10.478	C	-2.549	-0.717	-2.284
C	-0.878	-2.775	-9.063	O	-1.750	-1.348	-3.010
H	-1.429	-2.192	-9.812	O	-2.461	-0.596	-1.011
H	-1.616	-3.180	-8.360	N	-0.428	2.488	-8.929
C	0.089	-1.841	-8.317	C	-0.340	2.043	-10.184
H	0.651	-2.426	-7.579	H	0.018	1.021	-10.308
H	0.831	-1.438	-9.014	N	-0.615	2.689	-11.327
N	-0.542	-0.708	-7.652	C	-1.077	3.956	-11.276
H	-0.503	0.206	-8.088	N	-1.396	4.571	-12.436
C	-1.112	-0.746	-6.428	H	-1.133	4.095	-13.292
N	-1.265	-1.883	-5.750	H	-1.612	5.563	-12.454
H	-1.554	-1.802	-4.763	C	-1.210	4.553	-10.001
H	-0.996	-2.790	-6.115	N	-1.596	5.819	-9.601
N	-1.539	0.389	-5.862	C	-0.844	3.768	-8.898
H	-2.316	0.296	-5.168	N	-0.987	4.589	-7.800
H	-1.475	1.266	-6.363	C	-1.446	5.796	-8.298
C	-2.813	-7.653	-1.492	H	-1.645	6.632	-7.641
H	-2.286	-7.716	-0.531	C	-0.733	4.200	-6.414
H	-2.154	-7.153	-2.202	H	0.146	3.550	-6.422
O	-4.005	-6.895	-1.382	C	-0.479	5.381	-5.445
H	-4.614	-7.358	-0.772	H	-0.345	6.327	-5.983
N	-3.787	0.150	-4.220	O	0.655	5.071	-4.685
H	-4.633	0.663	-4.481	H	1.004	5.926	-4.313
H	-3.601	2.404	-4.178	C	-1.778	5.382	-4.591
C	-3.743	-0.029	-2.917	H	-2.574	5.866	-5.196
H	-4.305	0.602	-2.226	O	-1.694	6.055	-3.376
C	-5.177	-1.634	-2.448	H	-1.617	5.423	-2.626
H	-5.960	-1.027	-2.892	C	-2.091	3.883	-4.551
H	-5.120	-1.582	-1.365	H	-1.344	3.391	-3.912
C	-4.840	-2.857	-3.081	C	-3.483	3.484	-4.130
C	-4.376	-4.012	-2.441	H	-4.238	3.944	-4.779
H	-4.083	-4.164	-1.412	H	-3.658	3.796	-3.096
N	-4.334	-5.050	-3.317	O	-1.874	3.488	-5.933
H	-4.229	-6.009	-2.984				
C	-4.738	-4.621	-4.567	IM2-1			
C	-5.030	-3.232	-4.472	E=-2454.543646	$\Delta E=-0.192533$		
C	-5.396	-2.535	-5.630	C	-12.282	1.428	-4.486
H	-5.577	-1.465	-5.601	H	-12.671	0.671	-5.176
C	-5.481	-3.235	-6.831	H	-12.780	2.375	-4.727
H	-5.720	-2.685	-7.736	C	-10.789	1.636	-4.688

C	-9.832	0.618	-4.538	H	-4.205	-2.477	-1.871
H	-10.135	-0.369	-4.199	N	-4.369	-4.204	-3.128
C	-8.486	0.831	-4.817	H	-4.215	-4.959	-2.459
H	-7.752	0.042	-4.678	C	-4.681	-4.419	-4.456
C	-8.057	2.080	-5.289	C	-4.961	-3.161	-5.051
O	-6.742	2.218	-5.605	C	-5.307	-3.113	-6.408
H	-6.574	3.108	-5.983	H	-5.550	-2.164	-6.880
C	-10.332	2.888	-5.119	C	-5.348	-4.300	-7.136
H	-11.040	3.707	-5.234	H	-5.598	-4.281	-8.193
C	-8.989	3.113	-5.424	C	-4.764	-5.618	-5.171
H	-8.663	4.089	-5.773	H	-4.607	-6.568	-4.675
C	-0.191	-3.943	-9.561	C	-5.083	-5.540	-6.524
H	0.500	-4.428	-8.861	H	-5.143	-6.449	-7.113
H	0.431	-3.441	-10.314	C	-2.348	-0.266	-1.771
C	-1.010	-2.872	-8.827	O	-1.808	-0.609	-2.858
H	-1.590	-2.279	-9.543	O	-2.318	-0.904	-0.682
H	-1.719	-3.314	-8.117	N	-0.313	2.244	-8.931
C	-0.044	-1.934	-8.078	C	-0.277	1.708	-10.150
H	0.565	-2.522	-7.382	H	0.060	0.675	-10.217
H	0.657	-1.482	-8.788	N	-0.577	2.285	-11.324
N	-0.682	-0.841	-7.344	C	-0.993	3.565	-11.354
H	-0.696	0.078	-7.776	N	-1.309	4.120	-12.548
C	-1.013	-0.872	-6.031	H	-1.031	3.617	-13.389
N	-0.996	-2.019	-5.340	H	-1.459	5.118	-12.595
H	-1.202	-1.974	-4.345	C	-1.082	4.248	-10.124
H	-0.884	-2.931	-5.772	N	-1.417	5.550	-9.809
N	-1.365	0.252	-5.409	C	-0.703	3.531	-8.980
H	-1.632	0.190	-4.411	N	-0.792	4.429	-7.941
H	-1.237	1.167	-5.833	C	-1.231	5.611	-8.511
C	-3.014	-7.530	-1.898	H	-1.388	6.500	-7.917
H	-2.457	-7.454	-0.955	C	-0.461	4.119	-6.534
H	-2.412	-7.088	-2.690	H	0.534	3.674	-6.519
O	-4.243	-6.821	-1.840	C	-0.541	5.364	-5.635
H	-4.758	-7.193	-1.095	H	-0.270	6.283	-6.166
N	-2.764	2.049	-2.418	O	0.282	5.164	-4.520
H	-3.295	2.879	-2.137	H	0.763	6.012	-4.334
H	-3.651	2.197	-4.939	C	-2.038	5.315	-5.257
C	-3.083	1.058	-1.688	H	-2.600	5.558	-6.171
H	-3.818	1.103	-0.875	O	-2.497	6.198	-4.285
C	-5.075	-0.774	-4.142	H	-2.021	6.051	-3.428
H	-5.335	-0.335	-5.098	C	-2.221	3.815	-4.987
H	-4.976	-0.097	-3.303	H	-1.794	3.561	-4.013
C	-4.834	-2.146	-4.009	C	-3.627	3.276	-5.105
C	-4.456	-2.859	-2.851	H	-4.041	3.494	-6.095

H	-4.271	3.733	-4.351
O	-1.398	3.189	-6.023

TS3-1a

E=-2454.453520	$\Delta E=-0.200276$		
C	-12.358	1.459	-4.471
H	-12.746	0.703	-5.165
H	-12.869	2.403	-4.697
C	-10.871	1.683	-4.686
C	-9.912	0.663	-4.568
H	-10.208	-0.331	-4.248
C	-8.571	0.887	-4.854
H	-7.836	0.096	-4.740
C	-8.148	2.147	-5.300
O	-6.835	2.293	-5.620
H	-6.661	3.191	-5.977
C	-10.423	2.946	-5.092
H	-11.133	3.765	-5.183
C	-9.082	3.181	-5.402
H	-8.759	4.165	-5.731
C	-0.144	-3.944	-9.585
H	0.552	-4.422	-8.886
H	0.475	-3.444	-10.343
C	-0.965	-2.873	-8.856
H	-1.548	-2.280	-9.571
H	-1.673	-3.315	-8.146
C	0.003	-1.935	-8.108
H	0.635	-2.533	-7.440
H	0.683	-1.460	-8.823
N	-0.630	-0.863	-7.340
H	-0.557	0.089	-7.687
C	-1.076	-1.009	-6.069
N	-1.165	-2.204	-5.492
H	-1.531	-2.219	-4.530
H	-0.933	-3.080	-5.953
N	-1.457	0.066	-5.369
H	-1.757	-0.088	-4.399
H	-1.319	1.012	-5.709
C	-2.934	-7.466	-1.649
H	-2.372	-7.471	-0.704
H	-2.318	-6.985	-2.407
O	-4.138	-6.733	-1.539
H	-4.691	-7.180	-0.868
N	-2.609	1.357	-2.380

H	-2.668	2.291	-1.948
H	-3.665	2.131	-4.766
C	-3.315	0.487	-1.855
H	-4.035	0.522	-1.031
C	-5.236	-0.293	-4.288
H	-5.533	-0.100	-5.314
H	-5.275	0.557	-3.618
C	-4.838	-1.510	-3.885
C	-4.381	-1.894	-2.480
H	-5.056	-1.537	-1.694
N	-4.379	-3.360	-2.530
H	-3.905	-3.908	-1.825
C	-4.507	-3.814	-3.827
C	-4.811	-2.737	-4.691
C	-5.089	-2.976	-6.038
H	-5.358	-2.151	-6.695
C	-5.035	-4.284	-6.532
H	-5.244	-4.488	-7.580
C	-4.459	-5.131	-4.311
H	-4.288	-5.962	-3.636
C	-4.724	-5.345	-5.666
H	-4.704	-6.361	-6.051
C	-2.905	-1.363	-2.079
O	-2.030	-1.430	-3.026
O	-2.623	-1.535	-0.825
N	-0.294	2.144	-8.840
C	-0.236	1.615	-10.062
H	0.111	0.586	-10.130
N	-0.526	2.196	-11.236
C	-0.950	3.472	-11.267
N	-1.259	4.031	-12.460
H	-0.978	3.536	-13.306
H	-1.415	5.028	-12.502
C	-1.059	4.149	-10.034
N	-1.411	5.446	-9.718
C	-0.697	3.427	-8.887
N	-0.816	4.317	-7.843
C	-1.251	5.501	-8.417
H	-1.427	6.385	-7.823
C	-0.496	4.017	-6.432
H	0.493	3.559	-6.407
C	-0.566	5.279	-5.554
H	-0.291	6.186	-6.102
O	0.256	5.096	-4.436

H	0.741	5.945	-4.260
C	-2.063	5.239	-5.174
H	-2.629	5.432	-6.097
O	-2.529	6.160	-4.243
H	-2.046	6.060	-3.384
C	-2.237	3.748	-4.855
H	-1.763	3.530	-3.891
C	-3.649	3.215	-4.899
H	-4.129	3.459	-5.853
H	-4.235	3.657	-4.090
O	-1.449	3.104	-5.906

IM3-1a

E=-2454.484399 $\Delta E=-0.197362$

C	-12.322	1.440	-4.476
H	-12.714	0.686	-5.169
H	-12.824	2.388	-4.709
C	-10.832	1.651	-4.687
C	-9.879	0.625	-4.563
H	-10.184	-0.365	-4.238
C	-8.536	0.838	-4.850
H	-7.806	0.043	-4.731
C	-8.105	2.092	-5.305
O	-6.794	2.224	-5.635
H	-6.614	3.126	-5.980
C	-10.373	2.909	-5.096
H	-11.078	3.733	-5.189
C	-9.032	3.133	-5.408
H	-8.702	4.113	-5.742
C	-0.146	-3.941	-9.567
H	0.543	-4.424	-8.864
H	0.479	-3.445	-10.321
C	-0.966	-2.866	-8.842
H	-1.537	-2.268	-9.563
H	-1.685	-3.305	-8.141
C	-0.001	-1.933	-8.084
H	0.621	-2.532	-7.407
H	0.690	-1.463	-8.791
N	-0.639	-0.855	-7.328
H	-0.569	0.095	-7.684
C	-1.133	-0.998	-6.079
N	-1.243	-2.190	-5.497
H	-1.615	-2.199	-4.539
H	-0.965	-3.068	-5.929

N	-1.553	0.078	-5.401
H	-1.904	-0.080	-4.456
H	-1.399	1.028	-5.729
C	-2.957	-7.489	-1.747
H	-2.386	-7.457	-0.809
H	-2.354	-7.030	-2.530
O	-4.167	-6.759	-1.650
H	-4.705	-7.183	-0.951
N	-2.860	2.786	-1.837
H	-2.372	3.067	-0.962
H	-3.704	2.132	-4.817
C	-3.315	1.653	-1.968
H	-3.345	0.769	-1.314
C	-5.085	-0.483	-4.225
H	-5.389	-0.198	-5.228
H	-5.004	0.324	-3.504
C	-4.782	-1.753	-3.916
C	-4.328	-2.252	-2.534
H	-5.062	-2.002	-1.757
N	-4.254	-3.709	-2.725
H	-4.042	-4.379	-1.997
C	-4.529	-4.071	-4.018
C	-4.844	-2.928	-4.793
C	-5.163	-3.067	-6.144
H	-5.421	-2.190	-6.736
C	-5.160	-4.339	-6.728
H	-5.393	-4.465	-7.782
C	-4.559	-5.354	-4.587
H	-4.393	-6.230	-3.971
C	-4.863	-5.466	-5.945
H	-4.880	-6.453	-6.402
C	-2.951	-1.687	-2.060
O	-2.099	-1.398	-2.958
O	-2.774	-1.587	-0.819
N	-0.308	2.102	-8.843
C	-0.253	1.576	-10.067
H	0.084	0.544	-10.137
N	-0.534	2.162	-11.240
C	-0.946	3.443	-11.269
N	-1.247	4.007	-12.462
H	-0.969	3.513	-13.309
H	-1.395	5.005	-12.501
C	-1.049	4.118	-10.036
N	-1.386	5.419	-9.719

C	-0.697	3.391	-8.888
N	-0.808	4.281	-7.844
C	-1.229	5.470	-8.418
H	-1.399	6.354	-7.823
C	-0.485	3.980	-6.432
H	0.504	3.521	-6.412
C	-0.549	5.243	-5.557
H	-0.264	6.147	-6.107
O	0.270	5.052	-4.439
H	0.747	5.901	-4.245
C	-2.050	5.221	-5.186
H	-2.606	5.434	-6.112
O	-2.505	6.143	-4.251
H	-2.042	6.019	-3.384
C	-2.251	3.732	-4.874
H	-1.825	3.510	-3.892
C	-3.666	3.215	-4.959
H	-4.117	3.460	-5.927
H	-4.259	3.655	-4.157
O	-1.435	3.072	-5.902

TS3-1b

E=-2454.510608 $\Delta E=-0.194372$

C	-12.325	1.448	-4.466
H	-12.720	0.698	-5.161
H	-12.825	2.398	-4.694
C	-10.835	1.656	-4.680
C	-9.885	0.628	-4.561
H	-10.189	-0.361	-4.231
C	-8.545	0.835	-4.863
H	-7.823	0.032	-4.761
C	-8.111	2.085	-5.326
O	-6.805	2.208	-5.679
H	-6.625	3.113	-6.014
C	-10.374	2.911	-5.096
H	-11.077	3.738	-5.186
C	-9.035	3.130	-5.420
H	-8.705	4.108	-5.759
C	-0.155	-3.968	-9.589
H	0.534	-4.455	-8.889
H	0.469	-3.473	-10.344
C	-0.965	-2.891	-8.860
H	-1.544	-2.295	-9.576
H	-1.675	-3.324	-8.146

C	0.010	-1.957	-8.120
H	0.633	-2.549	-7.439
H	0.699	-1.495	-8.835
N	-0.625	-0.876	-7.368
H	-0.627	0.059	-7.767
C	-1.013	-0.966	-6.078
N	-1.008	-2.133	-5.426
H	-1.265	-2.120	-4.441
H	-0.849	-3.033	-5.872
N	-1.421	0.126	-5.428
H	-1.691	-0.008	-4.441
H	-1.284	1.062	-5.799
C	-2.990	-7.530	-1.850
H	-2.435	-7.465	-0.905
H	-2.389	-7.074	-2.634
O	-4.222	-6.828	-1.784
H	-4.742	-7.212	-1.049
N	-3.857	1.269	-2.741
H	-4.340	0.231	-3.331
H	-3.714	2.166	-5.060
C	-2.904	0.959	-1.975
H	-2.494	1.725	-1.298
C	-5.262	-0.722	-3.678
H	-5.592	-0.320	-4.638
H	-5.951	-0.439	-2.878
C	-4.888	-2.131	-3.694
C	-4.542	-2.915	-2.598
H	-4.374	-2.607	-1.575
N	-4.372	-4.224	-2.973
H	-4.221	-5.024	-2.354
C	-4.615	-4.339	-4.325
C	-4.911	-3.039	-4.825
C	-5.227	-2.902	-6.188
H	-5.492	-1.930	-6.596
C	-5.222	-4.032	-7.002
H	-5.445	-3.937	-8.062
C	-4.660	-5.483	-5.130
H	-4.500	-6.466	-4.701
C	-4.948	-5.314	-6.481
H	-4.982	-6.181	-7.134
C	-2.255	-0.419	-1.856
O	-1.851	-0.942	-2.934
O	-2.163	-0.905	-0.704
N	-0.302	2.143	-8.833

C	-0.251	1.610	-10.054
H	0.084	0.577	-10.119
N	-0.537	2.188	-11.230
C	-0.948	3.470	-11.264
N	-1.256	4.027	-12.458
H	-0.980	3.529	-13.303
H	-1.401	5.026	-12.501
C	-1.041	4.153	-10.034
N	-1.367	5.459	-9.726
C	-0.685	3.433	-8.883
N	-0.783	4.333	-7.845
C	-1.198	5.520	-8.426
H	-1.354	6.413	-7.839
C	-0.456	4.041	-6.430
H	0.540	3.598	-6.405
C	-0.550	5.299	-5.554
H	-0.261	6.208	-6.092
O	0.242	5.115	-4.415
H	0.740	5.956	-4.243
C	-2.057	5.264	-5.214
H	-2.594	5.490	-6.148
O	-2.535	6.172	-4.277
H	-2.067	6.061	-3.411
C	-2.272	3.768	-4.930
H	-1.908	3.534	-3.923
C	-3.676	3.252	-5.137
H	-4.046	3.550	-6.123
H	-4.342	3.635	-4.362
O	-1.388	3.115	-5.901

IM3-1b

E=-2454.543035	$\Delta E=-0.191314$		
C	-12.291	1.424	-4.483
H	-12.705	0.691	-5.186
H	-12.761	2.389	-4.705
C	-10.793	1.586	-4.686
C	-9.875	0.530	-4.558
H	-10.210	-0.452	-4.239
C	-8.523	0.701	-4.833
H	-7.828	-0.125	-4.723
C	-8.043	1.941	-5.276
O	-6.722	2.032	-5.579
H	-6.528	2.905	-5.987
C	-10.288	2.828	-5.091

H	-10.965	3.675	-5.190
C	-8.937	3.011	-5.389
H	-8.573	3.983	-5.711
C	-0.272	-3.970	-9.618
H	0.419	-4.432	-8.903
H	0.351	-3.477	-10.376
C	-1.103	-2.888	-8.915
H	-1.670	-2.302	-9.649
H	-1.822	-3.314	-8.206
C	-0.129	-1.955	-8.173
H	0.403	-2.523	-7.403
H	0.639	-1.595	-8.869
N	-0.735	-0.776	-7.554
H	-0.798	0.067	-8.109
C	-1.006	-0.607	-6.241
N	-1.036	-1.635	-5.391
H	-1.241	-1.466	-4.399
H	-1.014	-2.592	-5.722
N	-1.247	0.631	-5.801
H	-1.516	0.824	-4.833
H	-1.138	1.442	-6.398
C	-3.029	-7.559	-1.885
H	-2.474	-7.478	-0.941
H	-2.429	-7.108	-2.673
O	-4.268	-6.867	-1.823
H	-4.776	-7.244	-1.076
N	-2.175	1.528	-3.185
H	-3.676	2.703	-4.596
H	-3.911	-0.311	-4.562
C	-2.617	1.005	-2.150
H	-3.269	1.538	-1.446
C	-4.833	-0.772	-4.187
H	-5.621	-0.509	-4.901
H	-5.078	-0.276	-3.243
C	-4.710	-2.255	-4.024
C	-4.420	-2.961	-2.876
H	-4.212	-2.591	-1.881
N	-4.393	-4.315	-3.135
H	-4.271	-5.071	-2.460
C	-4.671	-4.516	-4.467
C	-4.862	-3.236	-5.065
C	-5.165	-3.170	-6.438
H	-5.333	-2.210	-6.920
C	-5.261	-4.352	-7.164

H	-5.482	-4.319	-8.227	C	-10.898	1.709	-4.678
C	-4.810	-5.707	-5.189	C	-9.948	0.678	-4.599
H	-4.715	-6.664	-4.692	H	-10.251	-0.325	-4.313
C	-5.090	-5.610	-6.548	C	-8.609	0.901	-4.888
H	-5.191	-6.512	-7.141	H	-7.893	0.090	-4.824
C	-2.187	-0.440	-1.733	C	-8.173	2.170	-5.289
O	-1.659	-1.153	-2.607	O	-6.859	2.313	-5.607
O	-2.409	-0.705	-0.521	H	-6.691	3.209	-5.973
N	-0.385	2.516	-8.881	C	-10.441	2.980	-5.044
C	-0.239	1.933	-10.071	H	-11.145	3.808	-5.108
H	0.185	0.929	-10.071	C	-9.099	3.215	-5.349
N	-0.516	2.430	-11.286	H	-8.771	4.207	-5.649
C	-1.031	3.671	-11.396	C	-0.193	-3.909	-9.547
N	-1.318	4.157	-12.623	H	0.499	-4.387	-8.843
H	-0.996	3.634	-13.437	H	0.429	-3.412	-10.303
H	-1.556	5.136	-12.715	C	-1.018	-2.833	-8.823
C	-1.249	4.395	-10.205	H	-1.588	-2.238	-9.546
N	-1.716	5.672	-9.966	H	-1.737	-3.272	-8.121
C	-0.867	3.766	-9.013	C	-0.052	-1.900	-8.066
N	-1.070	4.701	-8.025	H	0.557	-2.498	-7.378
C	-1.591	5.811	-8.666	H	0.650	-1.445	-8.773
H	-1.848	6.710	-8.124	N	-0.675	-0.804	-7.317
C	-0.721	4.494	-6.613	H	-0.623	0.133	-7.706
H	0.257	4.008	-6.599	C	-1.067	-0.892	-6.026
C	-0.685	5.801	-5.797	N	-1.147	-2.060	-5.396
H	-0.493	6.680	-6.421	H	-1.463	-2.047	-4.416
O	0.298	5.653	-4.810	H	-0.992	-2.955	-5.852
H	0.674	6.546	-4.600	N	-1.402	0.226	-5.361
C	-2.119	5.789	-5.214	H	-1.641	0.158	-4.374
H	-2.794	5.982	-6.063	H	-1.229	1.153	-5.740
O	-2.448	6.732	-4.245	C	-2.996	-7.477	-1.808
H	-2.047	6.475	-3.377	H	-2.424	-7.418	-0.871
C	-2.263	4.308	-4.847	H	-2.404	-7.019	-2.599
H	-1.636	4.096	-3.972	O	-4.222	-6.769	-1.718
C	-3.662	3.792	-4.614	H	-4.746	-7.190	-1.006
H	-4.356	4.129	-5.388	N	-2.618	1.727	-2.740
H	-4.017	4.151	-3.643	H	-3.654	2.346	-5.048
O	-1.686	3.644	-6.010	H	-4.251	-0.001	-4.524
TS4-1b				C	-3.348	2.217	-1.990
E=-2454.496302 $\Delta E=-0.195283$				H	-4.009	2.681	-1.289
C	-12.383	1.482	-4.462	C	-5.098	-0.465	-3.999
H	-12.770	0.731	-5.162	H	-5.976	-0.290	-4.628
H	-12.896	2.427	-4.680	H	-5.239	0.083	-3.065
				C	-4.867	-1.919	-3.758

C	-4.508	-2.511	-2.515
H	-4.866	-2.192	-1.541
N	-4.358	-3.892	-2.743
H	-4.231	-4.616	-2.043
C	-4.565	-4.176	-4.074
C	-4.861	-2.943	-4.741
C	-5.146	-2.974	-6.125
H	-5.404	-2.057	-6.650
C	-5.142	-4.196	-6.795
H	-5.366	-4.232	-7.860
C	-4.590	-5.402	-4.743
H	-4.442	-6.328	-4.200
C	-4.873	-5.399	-6.114
H	-4.904	-6.341	-6.655
C	-2.686	-1.446	-1.911
O	-1.784	-1.373	-2.770
O	-2.744	-1.009	-0.745
N	-0.308	2.241	-8.858
C	-0.251	1.670	-10.061
H	0.093	0.637	-10.093
N	-0.537	2.207	-11.257
C	-0.961	3.482	-11.331
N	-1.257	4.012	-12.540
H	-0.967	3.502	-13.375
H	-1.416	5.008	-12.601
C	-1.078	4.198	-10.123
N	-1.426	5.507	-9.861
C	-0.708	3.524	-8.951
N	-0.812	4.461	-7.946
C	-1.252	5.620	-8.566
H	-1.420	6.531	-8.012
C	-0.451	4.230	-6.530
H	0.556	3.813	-6.509
C	-0.556	5.521	-5.702
H	-0.291	6.414	-6.277
O	0.258	5.395	-4.570
H	0.703	6.268	-4.419
C	-2.057	5.471	-5.338
H	-2.612	5.680	-6.264
O	-2.531	6.382	-4.397
H	-2.089	6.232	-3.523
C	-2.241	3.980	-5.012
H	-1.873	3.792	-3.999
C	-3.634	3.426	-5.200

H	-3.999	3.644	-6.209
H	-4.325	3.865	-4.477
O	-1.347	3.302	-5.948

IM4-1b

E=-2454.529111 $\Delta E=-0.197025$			
C	-12.384	1.474	-4.457
H	-12.765	0.719	-5.154
H	-12.901	2.416	-4.681
C	-10.899	1.708	-4.666
C	-9.940	0.688	-4.559
H	-10.237	-0.313	-4.259
C	-8.598	0.919	-4.834
H	-7.872	0.121	-4.741
C	-8.171	2.187	-5.252
O	-6.854	2.340	-5.553
H	-6.692	3.230	-5.937
C	-10.450	2.978	-5.049
H	-11.161	3.797	-5.134
C	-9.107	3.221	-5.344
H	-8.786	4.210	-5.656
C	-0.169	-3.917	-9.548
H	0.521	-4.398	-8.845
H	0.455	-3.421	-10.303
C	-0.991	-2.842	-8.823
H	-1.553	-2.238	-9.545
H	-1.717	-3.281	-8.129
C	-0.025	-1.922	-8.051
H	0.576	-2.530	-7.364
H	0.684	-1.464	-8.749
N	-0.648	-0.829	-7.299
H	-0.568	0.114	-7.669
C	-1.095	-0.935	-6.026
N	-1.224	-2.108	-5.418
H	-1.611	-2.115	-4.457
H	-1.014	-2.995	-5.870
N	-1.442	0.180	-5.361
H	-1.713	0.111	-4.383
H	-1.255	1.107	-5.728
C	-2.980	-7.455	-1.769
H	-2.407	-7.405	-0.833
H	-2.386	-6.995	-2.558
O	-4.201	-6.740	-1.674
H	-4.731	-7.166	-0.971

N	-2.606	1.561	-2.832	O	0.260	5.364	-4.542
H	-3.656	2.342	-5.052	H	0.712	6.234	-4.392
H	-4.246	0.162	-4.425	C	-2.048	5.457	-5.329
C	-3.310	2.076	-2.075	H	-2.596	5.666	-6.259
H	-3.939	2.566	-1.361	O	-2.526	6.372	-4.394
C	-5.136	-0.414	-4.140	H	-2.088	6.226	-3.517
H	-5.829	-0.344	-4.984	C	-2.241	3.968	-5.001
H	-5.589	0.106	-3.288	H	-1.880	3.780	-3.985
C	-4.814	-1.833	-3.829	C	-3.636	3.422	-5.196
C	-4.350	-2.336	-2.478	H	-3.996	3.645	-6.206
H	-5.084	-2.135	-1.680	H	-4.328	3.857	-4.473
N	-4.211	-3.776	-2.721	O	-1.347	3.284	-5.931
H	-4.068	-4.479	-2.006				
C	-4.506	-4.104	-4.017	TS2-2			
C	-4.845	-2.903	-4.735	E=-2454.509922	ΔE=-0.198929		
C	-5.177	-2.995	-6.109	C	-12.272	1.405	-4.458
H	-5.448	-2.100	-6.665	H	-12.676	0.666	-5.160
C	-5.167	-4.242	-6.734	H	-12.742	2.368	-4.693
H	-5.401	-4.324	-7.793	C	-10.772	1.569	-4.644
C	-4.554	-5.354	-4.637	C	-9.852	0.513	-4.515
H	-4.384	-6.257	-4.065	H	-10.188	-0.470	-4.200
C	-4.867	-5.408	-6.005	C	-8.502	0.685	-4.797
H	-4.886	-6.372	-6.507	H	-7.809	-0.146	-4.713
C	-2.998	-1.671	-1.994	C	-8.024	1.927	-5.236
O	-2.053	-1.622	-2.833	O	-6.705	2.021	-5.549
O	-2.946	-1.243	-0.807	H	-6.512	2.906	-5.929
N	-0.302	2.219	-8.843	C	-10.269	2.812	-5.046
C	-0.250	1.649	-10.047	H	-10.947	3.657	-5.149
H	0.089	0.615	-10.081	C	-8.918	2.997	-5.343
N	-0.535	2.190	-11.242	H	-8.558	3.967	-5.673
C	-0.953	3.467	-11.313	C	-0.211	-3.915	-9.577
N	-1.250	4.000	-12.521	H	0.488	-4.387	-8.876
H	-0.963	3.492	-13.357	H	0.404	-3.407	-10.332
H	-1.404	4.997	-12.580	C	-1.047	-2.855	-8.847
C	-1.064	4.182	-10.104	H	-1.649	-2.278	-9.561
N	-1.404	5.493	-9.840	H	-1.741	-3.306	-8.129
C	-0.696	3.504	-8.933	C	-0.088	-1.893	-8.116
N	-0.797	4.440	-7.927	H	0.555	-2.471	-7.441
C	-1.230	5.602	-8.545	H	0.583	-1.418	-8.839
H	-1.393	6.513	-7.989	N	-0.733	-0.818	-7.360
C	-0.442	4.206	-6.510	H	-0.695	0.123	-7.741
H	0.561	3.782	-6.484	C	-1.144	-0.928	-6.074
C	-0.544	5.497	-5.681	N	-1.171	-2.104	-5.455
H	-0.268	6.388	-6.253	H	-1.438	-2.151	-4.458

H	-0.952	-2.978	-5.925
N	-1.529	0.178	-5.423
H	-1.931	0.154	-4.479
H	-1.490	1.095	-5.858
C	-3.041	-7.563	-1.790
H	-2.485	-7.505	-0.845
H	-2.446	-7.088	-2.568
O	-4.283	-6.882	-1.710
H	-4.793	-7.282	-0.978
N	-3.005	0.706	-2.824
H	-2.625	1.078	-1.946
H	-3.900	2.243	-4.613
C	-4.050	0.013	-2.588
H	-4.433	-0.128	-1.570
C	-4.846	-0.647	-3.684
H	-4.490	-0.270	-4.650
H	-5.887	-0.299	-3.580
C	-4.757	-2.152	-3.642
C	-4.462	-2.935	-2.505
H	-4.691	-2.706	-1.471
N	-4.437	-4.272	-2.895
H	-4.332	-5.080	-2.281
C	-4.628	-4.364	-4.253
C	-4.825	-3.037	-4.757
C	-5.063	-2.876	-6.140
H	-5.242	-1.887	-6.556
C	-5.093	-4.002	-6.961
H	-5.270	-3.883	-8.028
C	-4.687	-5.492	-5.074
H	-4.583	-6.486	-4.651
C	-4.913	-5.299	-6.441
H	-4.963	-6.160	-7.102
C	-2.428	-2.225	-1.848
O	-1.565	-2.071	-2.731
O	-2.407	-2.073	-0.619
N	-0.343	2.273	-8.821
C	-0.271	1.827	-10.076
H	0.079	0.804	-10.206
N	-0.556	2.481	-11.213
C	-0.999	3.753	-11.158
N	-1.336	4.367	-12.316
H	-1.079	3.898	-13.179
H	-1.521	5.362	-12.327
C	-1.102	4.354	-9.882

N	-1.466	5.624	-9.473
C	-0.740	3.557	-8.786
N	-0.866	4.373	-7.682
C	-1.309	5.589	-8.170
H	-1.490	6.426	-7.509
C	-0.634	3.949	-6.297
H	0.277	3.347	-6.291
C	-0.504	5.122	-5.300
H	-0.266	6.059	-5.814
O	0.484	4.807	-4.358
H	0.911	5.661	-4.078
C	-1.920	5.152	-4.667
H	-2.599	5.633	-5.398
O	-2.046	5.864	-3.477
H	-1.837	5.284	-2.711
C	-2.268	3.658	-4.621
H	-1.707	3.190	-3.802
C	-3.734	3.315	-4.520
H	-4.309	3.832	-5.294
H	-4.109	3.622	-3.540
O	-1.746	3.155	-5.883

IM2-2

E=-2454.538991	ΔE=-0.199538		
C	-12.284	1.406	-4.459
H	-12.680	0.662	-5.160
H	-12.761	2.364	-4.696
C	-10.785	1.582	-4.643
C	-9.861	0.529	-4.530
H	-10.192	-0.460	-4.233
C	-8.511	0.713	-4.808
H	-7.815	-0.117	-4.741
C	-8.039	1.965	-5.223
O	-6.718	2.074	-5.529
H	-6.532	2.968	-5.893
C	-10.288	2.835	-5.024
H	-10.971	3.677	-5.116
C	-8.938	3.032	-5.315
H	-8.583	4.009	-5.629
C	-0.188	-3.897	-9.574
H	0.513	-4.369	-8.875
H	0.423	-3.384	-10.327
C	-1.032	-2.845	-8.838
H	-1.620	-2.255	-9.552

H	-1.737	-3.305	-8.137	N	-0.377	2.314	-8.839
C	-0.083	-1.900	-8.075	C	-0.313	1.849	-10.088
H	0.533	-2.489	-7.385	H	0.019	0.818	-10.203
H	0.615	-1.431	-8.778	N	-0.584	2.491	-11.235
N	-0.732	-0.816	-7.335	C	-1.005	3.772	-11.200
H	-0.679	0.120	-7.723	N	-1.330	4.375	-12.366
C	-1.184	-0.908	-6.060	H	-1.081	3.891	-13.223
N	-1.250	-2.074	-5.427	H	-1.505	5.372	-12.388
H	-1.599	-2.133	-4.448	C	-1.094	4.393	-9.934
H	-0.995	-2.947	-5.878	N	-1.429	5.678	-9.546
N	-1.578	0.217	-5.443	C	-0.749	3.607	-8.824
H	-1.979	0.225	-4.497	N	-0.857	4.445	-7.734
H	-1.529	1.119	-5.905	C	-1.271	5.663	-8.242
C	-2.978	-7.522	-1.777	H	-1.437	6.515	-7.596
H	-2.421	-7.471	-0.832	C	-0.661	4.036	-6.342
H	-2.376	-7.057	-2.556	H	0.229	3.402	-6.312
O	-4.208	-6.820	-1.699	C	-0.500	5.215	-5.355
H	-4.731	-7.222	-0.976	H	-0.265	6.148	-5.879
N	-2.991	0.811	-2.875	O	0.507	4.895	-4.436
H	-2.617	1.214	-2.007	H	0.923	5.750	-4.143
H	-3.908	2.377	-4.607	C	-1.902	5.265	-4.691
C	-4.085	0.206	-2.633	H	-2.592	5.753	-5.406
H	-4.499	0.142	-1.619	O	-1.992	5.977	-3.498
C	-4.863	-0.519	-3.701	H	-1.797	5.388	-2.735
H	-4.557	-0.148	-4.687	C	-2.263	3.774	-4.641
H	-5.923	-0.242	-3.577	H	-1.666	3.293	-3.856
C	-4.684	-2.009	-3.618	C	-3.725	3.440	-4.467
C	-4.256	-2.734	-2.365	H	-4.348	4.002	-5.169
H	-4.933	-2.574	-1.510	H	-4.033	3.700	-3.450
N	-4.276	-4.129	-2.790	O	-1.810	3.287	-5.935
H	-4.129	-4.928	-2.177				
C	-4.567	-4.248	-4.114	TS3-2			
C	-4.823	-2.938	-4.661	E=-2454.448767	ΔE=-0.203309		
C	-5.156	-2.825	-6.033	C	-12.312	1.381	-4.446
H	-5.373	-1.850	-6.464	H	-12.712	0.633	-5.141
C	-5.207	-3.977	-6.819	H	-12.789	2.339	-4.687
H	-5.434	-3.899	-7.879	C	-10.814	1.552	-4.636
C	-4.665	-5.398	-4.901	C	-9.887	0.506	-4.486
H	-4.524	-6.378	-4.459	H	-10.215	-0.473	-4.153
C	-4.970	-5.247	-6.262	C	-8.537	0.685	-4.762
H	-5.027	-6.131	-6.893	H	-7.831	-0.133	-4.647
C	-2.817	-2.293	-1.882	C	-8.073	1.923	-5.222
O	-1.921	-2.219	-2.766	O	-6.754	2.023	-5.538
O	-2.677	-2.051	-0.659	H	-6.562	2.919	-5.894

C	-10.322	2.794	-5.053
H	-11.007	3.632	-5.168
C	-8.972	2.986	-5.348
H	-8.617	3.955	-5.689
C	-0.166	-4.004	-9.632
H	0.541	-4.485	-8.945
H	0.440	-3.491	-10.390
C	-0.979	-2.948	-8.878
H	-1.578	-2.349	-9.575
H	-1.670	-3.397	-8.155
C	0.008	-2.020	-8.146
H	0.645	-2.621	-7.485
H	0.683	-1.554	-8.872
N	-0.609	-0.943	-7.382
H	-0.527	0.004	-7.738
C	-1.042	-1.051	-6.102
N	-1.079	-2.220	-5.468
H	-1.471	-2.273	-4.513
H	-0.819	-3.097	-5.912
N	-1.447	0.053	-5.473
H	-1.702	0.059	-4.462
H	-1.442	0.955	-5.935
C	-2.958	-7.383	-1.761
H	-2.393	-7.335	-0.821
H	-2.359	-6.924	-2.545
O	-4.180	-6.666	-1.674
H	-4.705	-7.075	-0.958
N	-2.264	0.627	-2.898
H	-1.695	1.037	-2.151
H	-3.780	1.994	-3.838
C	-3.494	0.923	-2.818
H	-3.946	1.478	-1.984
C	-4.994	-0.311	-3.613
H	-5.229	0.116	-4.586
H	-5.679	0.040	-2.841
C	-4.676	-1.704	-3.561
C	-4.296	-2.438	-2.294
H	-4.919	-2.174	-1.429
N	-4.442	-3.842	-2.670
H	-4.180	-4.626	-2.077
C	-4.547	-3.966	-4.022
C	-4.705	-2.666	-4.615
C	-4.948	-2.581	-6.002
H	-5.127	-1.614	-6.464

C	-4.970	-3.745	-6.768
H	-5.127	-3.684	-7.842
C	-4.591	-5.137	-4.793
H	-4.505	-6.108	-4.318
C	-4.792	-5.010	-6.169
H	-4.827	-5.907	-6.784
C	-2.788	-2.161	-1.901
O	-1.943	-2.378	-2.803
O	-2.562	-1.789	-0.724
N	-0.338	2.207	-8.728
C	-0.240	1.776	-9.987
H	0.123	0.759	-10.123
N	-0.513	2.440	-11.121
C	-0.964	3.708	-11.058
N	-1.301	4.330	-12.212
H	-1.040	3.873	-13.080
H	-1.488	5.324	-12.216
C	-1.082	4.296	-9.779
N	-1.458	5.561	-9.365
C	-0.745	3.487	-8.682
N	-0.906	4.291	-7.571
C	-1.337	5.511	-8.059
H	-1.535	6.342	-7.396
C	-0.733	3.861	-6.180
H	0.178	3.259	-6.138
C	-0.632	5.031	-5.168
H	-0.453	5.984	-5.675
O	0.394	4.756	-4.257
H	0.835	5.616	-4.024
C	-2.033	4.989	-4.496
H	-2.750	5.477	-5.183
O	-2.145	5.637	-3.271
H	-1.885	5.033	-2.541
C	-2.320	3.479	-4.495
H	-1.668	3.019	-3.736
C	-3.751	3.056	-4.259
H	-4.353	3.102	-5.169
H	-4.187	3.691	-3.483
O	-1.866	3.065	-5.813

IM3-2

E=-2454.465452 ΔE =-0.198279

C	-12.303	1.413	-4.457
H	-12.701	0.668	-5.157

H	-12.783	2.370	-4.692	C	-4.914	-2.057	-3.472
C	-10.806	1.592	-4.645	C	-4.392	-2.872	-2.288
C	-9.876	0.548	-4.501	H	-5.030	-2.801	-1.400
H	-10.201	-0.435	-4.175	N	-4.356	-4.232	-2.818
C	-8.526	0.732	-4.773	H	-4.219	-5.070	-2.257
H	-7.822	-0.085	-4.653	C	-4.563	-4.246	-4.163
C	-8.061	1.975	-5.223	C	-4.839	-2.933	-4.640
O	-6.740	2.081	-5.530	C	-5.122	-2.727	-5.990
H	-6.553	2.970	-5.901	H	-5.361	-1.728	-6.347
C	-10.315	2.837	-5.054	C	-5.111	-3.814	-6.870
H	-11.002	3.675	-5.165	H	-5.301	-3.662	-7.929
C	-8.965	3.034	-5.345	C	-4.604	-5.347	-5.036
H	-8.613	4.006	-5.680	H	-4.458	-6.353	-4.658
C	-0.202	-3.953	-9.593	C	-4.865	-5.111	-6.387
H	0.506	-4.427	-8.902	H	-4.891	-5.956	-7.072
H	0.403	-3.433	-10.348	C	-2.956	-2.380	-1.892
C	-1.036	-2.906	-8.845	O	-2.101	-2.345	-2.818
H	-1.630	-2.308	-9.547	O	-2.763	-2.061	-0.691
H	-1.735	-3.367	-8.137	N	-0.348	2.268	-8.808
C	-0.070	-1.974	-8.090	C	-0.280	1.810	-10.059
H	0.546	-2.570	-7.406	H	0.064	0.784	-10.179
H	0.628	-1.514	-8.799	N	-0.561	2.454	-11.202
N	-0.703	-0.886	-7.350	C	-0.995	3.730	-11.160
H	-0.624	0.054	-7.724	N	-1.327	4.335	-12.324
C	-1.170	-0.981	-6.081	H	-1.071	3.859	-13.183
N	-1.239	-2.145	-5.444	H	-1.504	5.331	-12.342
H	-1.647	-2.206	-4.493	C	-1.093	4.344	-9.890
H	-0.963	-3.020	-5.881	N	-1.445	5.622	-9.494
N	-1.580	0.141	-5.476	C	-0.738	3.556	-8.785
H	-1.834	0.166	-4.482	N	-0.859	4.384	-7.690
H	-1.504	1.047	-5.927	C	-1.290	5.599	-8.190
C	-2.986	-7.566	-1.784	H	-1.465	6.444	-7.539
H	-2.433	-7.519	-0.836	C	-0.645	3.967	-6.300
H	-2.385	-7.088	-2.556	H	0.271	3.373	-6.278
O	-4.223	-6.878	-1.706	C	-0.534	5.142	-5.301
H	-4.740	-7.276	-0.977	H	-0.318	6.086	-5.811
N	-2.215	0.904	-2.737	O	0.465	4.842	-4.365
H	-1.504	1.237	-2.068	H	0.890	5.698	-4.091
H	-3.850	2.176	-4.561	C	-1.947	5.143	-4.657
C	-3.326	0.613	-2.277	H	-2.639	5.626	-5.374
H	-3.744	0.646	-1.266	O	-2.072	5.833	-3.455
C	-5.385	-0.795	-3.381	H	-1.848	5.244	-2.700
H	-5.674	-0.224	-4.258	C	-2.265	3.643	-4.624
H	-5.655	-0.366	-2.423	H	-1.678	3.184	-3.819

C	-3.718	3.256	-4.491
H	-4.327	3.736	-5.263
H	-4.085	3.571	-3.510
O	-1.757	3.167	-5.901