

Supporting Information available for

**A theoretical study based on DFT calculations on the
different influence of functional groups on the C-H
activation process via Pd-catalyzed β -X elimination**

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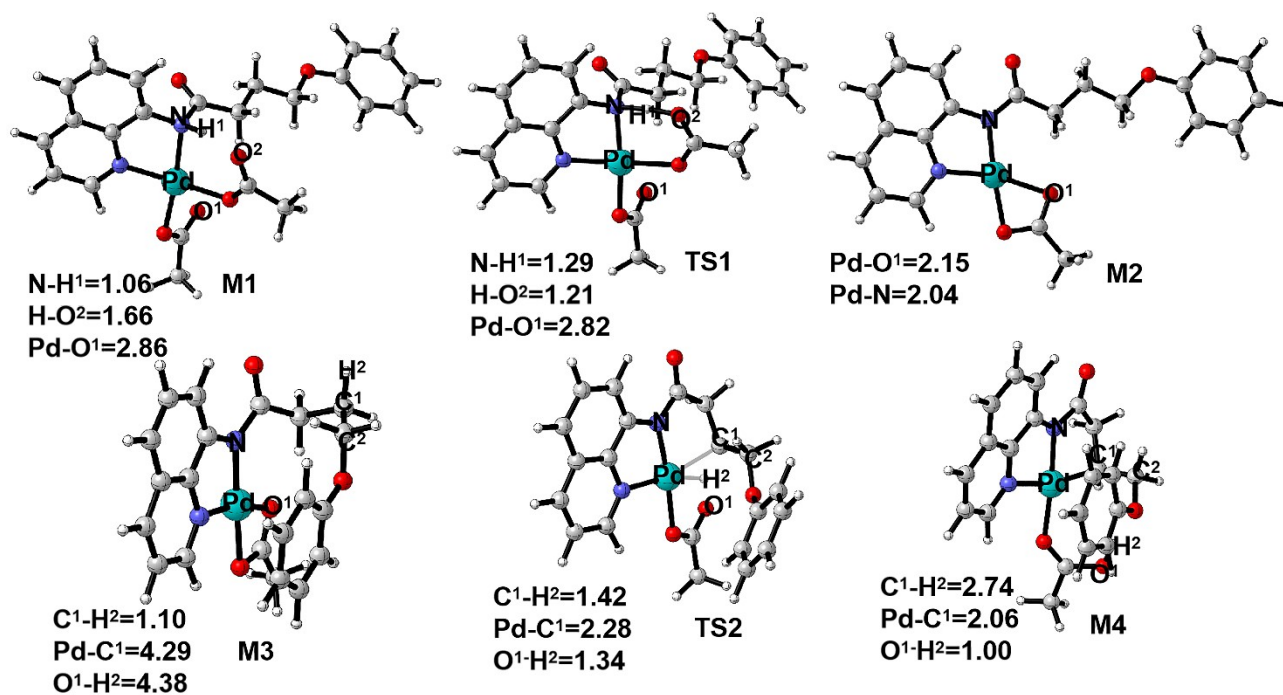
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B3LYP combined with DFT-D3(BJ) dispersion correction, called B3LYP-D3(BJ), is very reasonable for the description of systems involving weak interactions, and has still been widely used in many recent studies. "B3LYP, still have an important role to play in the search for transition state geometries for organic reactions, and can generate results that are almost as reliable as much more expensive computational method. [1]"

[1] Goodman, L. S. o. J. M. (2011). "How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals." *Organic & Biomolecular Chemistry* **9**: 689.

Fig. S1 The geometric structures for the intermediate **M1**, **M2**, **M3**, **M4** and the transition state **TS1**, **TS2** and some important bond lengths (in Å).



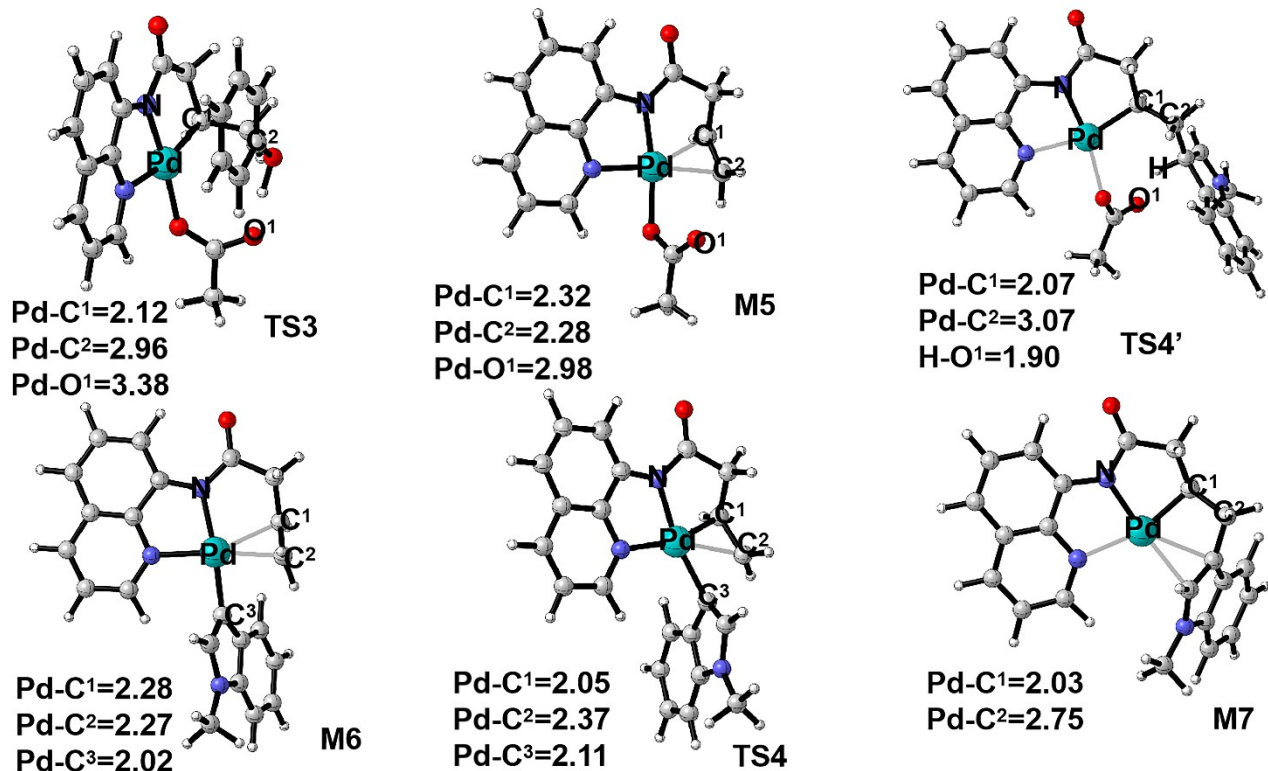


Fig. S2 The geometric structures for the intermediate M5, M6, M7 and the transition state TS3, TS4', Ts4 and some important bond lengths (in Å).

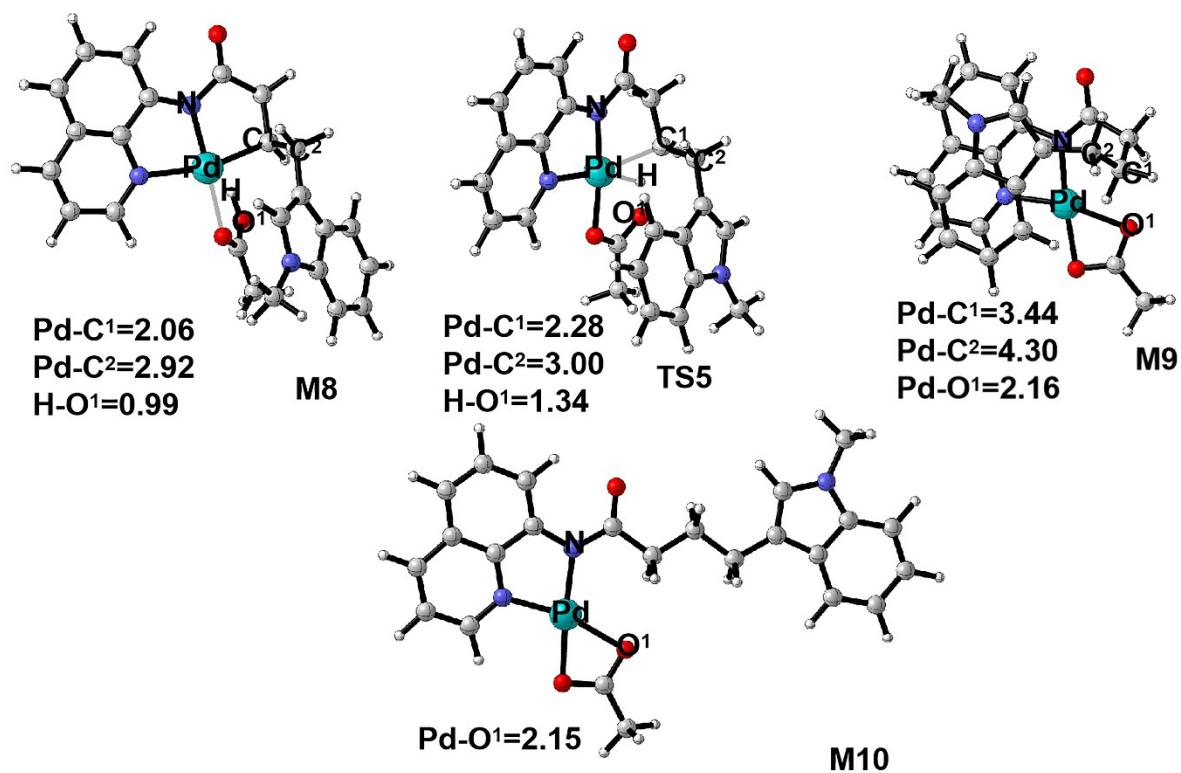


Fig. S3 The geometric structures for the intermediate M8, M9, M10 and the transition state TS5 and some important bond lengths (in Å).

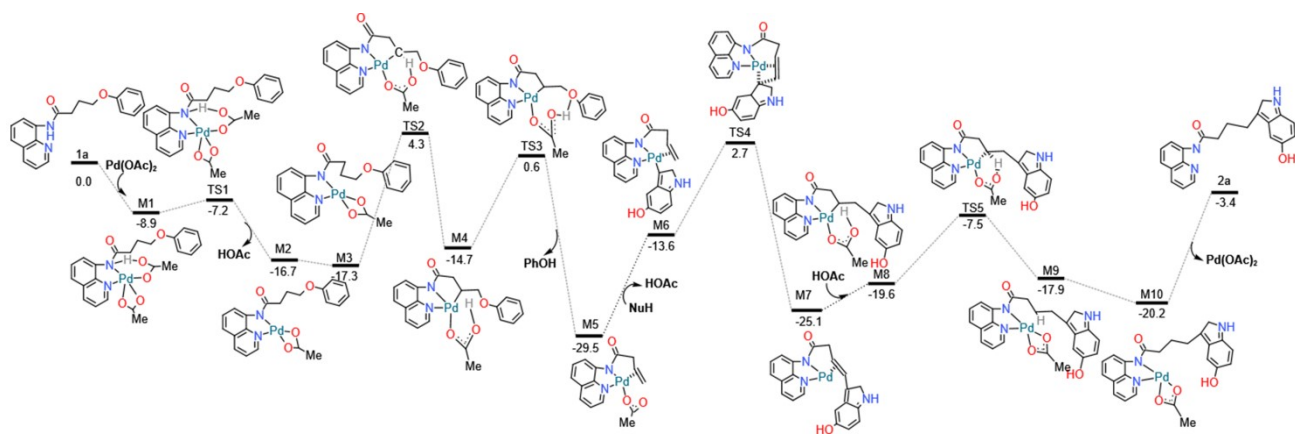


Fig. S4 Overview of free energy for 2A-OH catalytic activation.

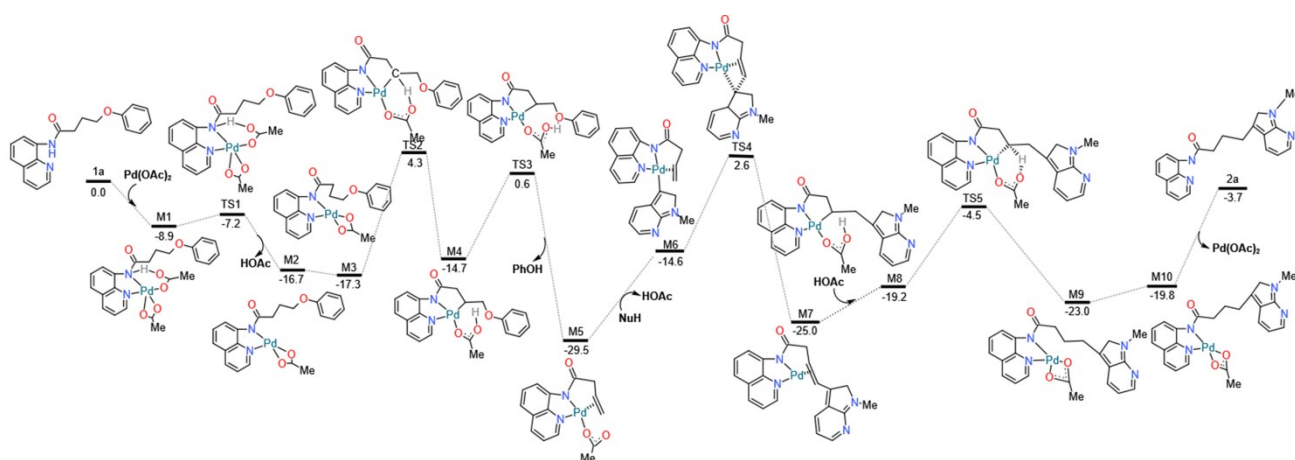


Fig. S5 Overview of free energy for N-2A catalytic activation.

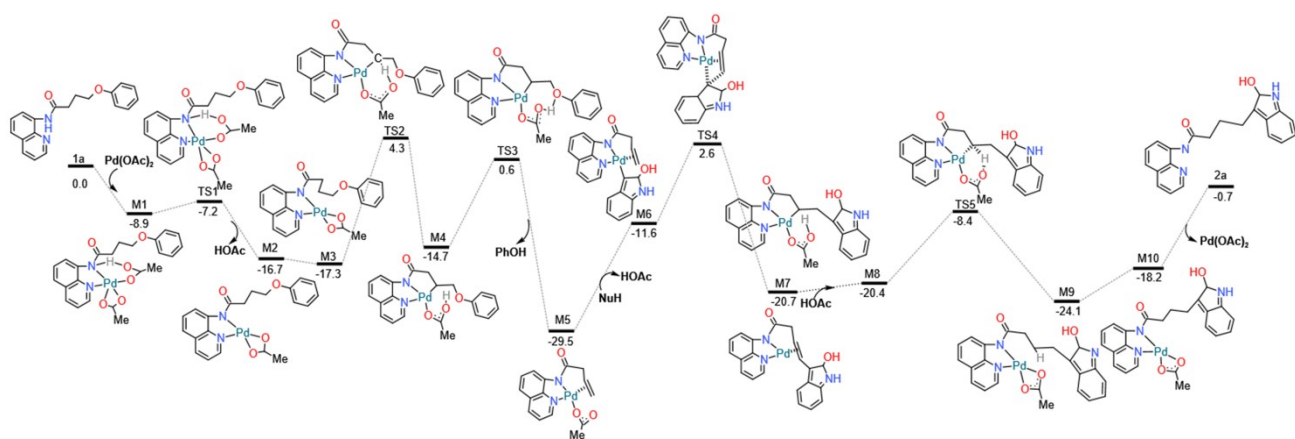


Fig. S6 Overview of free energy for HO-2A catalytic activation.

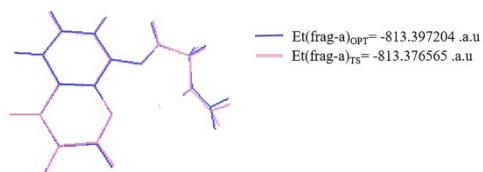


Fig. S7 The geometry and the Et(frag-a)TS, and Et(frag-a)opt energy value of the fragment a.

The example of deformation energy analysis:

$$\Delta E_{tot} = E(TS4) - E(Frag_a) - E(Frag_b) = -0.080142 \text{ a.u.} = -50.49 \text{ kcal mol}^{-1}$$

$$\Delta E_{orb} = E_SCF_last - E_SCF_1st = -0.002079 \text{ a.u.} = -1.31 \text{ kcal mol}^{-1}$$

$$\Delta E_{steric} = \Delta E_{els} + \Delta E_{ex} = \Delta E_{tot} - \Delta E_{orb} = -0.078063 \text{ a.u.} = -49.18 \text{ kcal mol}^{-1}$$

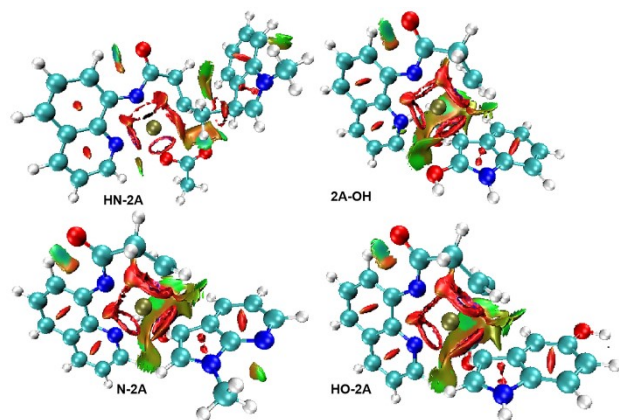


Fig. S8 The Non-Covalent Interactions for the steric interaction of geometry TS4 of different nucleophile groups.

Cartesian coordinates for all of the calculated structures.

Pd(OAc)₂

SCF Done: -583.750577 .a.u

Pd	0.693141	1.231187	0.040553
O	1.405068	0.918228	1.970209
O	0.255482	-0.603109	0.919284
O	-0.018393	1.544261	-1.889022
O	1.130848	3.065142	-0.838412
C	0.887481	-0.251635	1.974526
C	0.498955	2.713968	-1.893529
C	0.345473	3.635867	-3.060194

H	0.248457	3.059388	-3.982917
H	-0.565110	4.231544	-2.926439
H	1.198233	4.316302	-3.114653
C	1.041130	-1.173624	3.141139
H	1.137837	-0.596986	4.063820
H	0.188137	-1.853799	3.195626
H	1.951649	-1.769490	3.007728

Sub-HN-2A

SCF Done: -403.141432 .a.u

C	-1.701807	2.432016	0.042703
C	-3.125729	2.429421	0.065912
C	-3.804224	3.659199	0.025367
C	-3.067602	4.835949	-0.035827
C	-1.657323	4.814024	-0.057780
C	-0.955318	3.614012	-0.018987
C	-2.391277	0.299739	0.143042
C	-3.534432	1.054853	0.129967
H	-4.890841	3.686157	0.041836
H	-3.583585	5.791838	-0.067440
H	-1.109564	5.751277	-0.105884
H	0.130897	3.596487	-0.035937
H	-2.266273	-0.774100	0.185982
H	-4.547182	0.677380	0.162143
C	0.106654	0.692631	0.086502
H	0.615462	1.023849	-0.826890
H	0.644060	1.099368	0.951721
H	0.146703	-0.397959	0.132164
N	-1.275893	1.118815	0.090698

Sub-2A-OH

SCF Done: -439.040585 .a.u

C	-1.768403	2.408797	-0.021313
C	-3.191967	2.394304	-0.033639
C	-3.891598	3.610404	-0.092931
C	-3.168064	4.795970	-0.138081
C	-1.755509	4.792539	-0.125105
C	-1.042579	3.599871	-0.066607
C	-2.448076	0.263184	0.066300
C	-3.593025	1.016480	0.022958
H	-4.976197	3.646848	-0.104348
H	-1.219384	5.739058	-0.161621
H	0.044119	3.604213	-0.056755
H	-2.323932	-0.809940	0.114111
H	-4.604990	0.635980	0.030243
H	-0.384500	0.788899	0.061932
N	-1.344559	1.092884	0.040242
O	-3.882948	5.970424	-0.195778
H	-3.261631	6.713311	-0.222715

Sub-N-2A

SCF Done: -419.185636 .a.u

C	-1.749449	2.450428	0.056137
C	-3.175741	2.419639	0.032396
C	-3.826417	3.659797	0.032284
C	-3.035938	4.805482	0.055063
C	-1.632515	4.692703	0.077171
C	-2.394969	0.309780	0.027260
C	-3.557449	1.039367	0.014350

H	-4.911312	3.726389	0.015026
H	-3.489907	5.791801	0.056036
H	-1.017345	5.590397	0.095007
H	-2.251837	-0.762541	0.020487
H	-4.560702	0.636576	-0.005584
C	0.098624	0.746390	0.071919
H	0.348482	0.163665	-0.821693
H	0.705231	1.653225	0.090074
H	0.318995	0.147656	0.962699
N	-1.295175	1.147667	0.052513
N	-0.970456	3.531176	0.078146

Sub-HO-2A

SCF Done: -439.042837 .a.u

C	-1.686816	2.484262	0.137639
C	-3.109606	2.438195	0.099107
C	-3.814269	3.643544	-0.040325
C	-3.104589	4.837614	-0.136152
C	-1.698434	4.856011	-0.095538
C	-0.970028	3.675385	0.042439
C	-2.331634	0.340718	0.328467
C	-3.497213	1.057238	0.223017
H	-4.900753	3.641996	-0.072907
H	-3.645464	5.774019	-0.244395
H	-1.170773	5.802539	-0.172580
H	0.116451	3.683291	0.074515
H	-4.500593	0.654099	0.232038
H	-0.285310	0.864060	0.337806
N	-1.241580	1.177293	0.279593

O	-2.072269	-0.983291	0.466071
H	-2.917868	-1.456041	0.486782

1a

SCF Done: -994.926468 .a.u

C	-13.300229	-0.897296	0.222386
C	-11.988089	-1.278614	0.001423
C	-10.958212	-0.280985	-0.053109
C	-11.300988	1.092776	0.121314
C	-12.654077	1.451415	0.345381
C	-13.617793	0.470055	0.391978
H	-14.069629	-1.654744	0.263222
C	-10.240060	2.029849	0.057272
H	-12.911460	2.498459	0.477949
H	-14.655695	0.740205	0.563820
C	-8.954469	1.593151	-0.164385
C	-8.725526	0.206520	-0.324054
H	-10.458591	3.087041	0.185157
H	-8.122479	2.287927	-0.218149
H	-7.716266	-0.161559	-0.500493
N	-9.681629	-0.700738	-0.272177
N	-11.546877	-2.590784	-0.179825
H	-10.542940	-2.640701	-0.328378
C	-12.287309	-3.745684	-0.200391
O	-13.498131	-3.786252	-0.024604
C	-11.466888	-4.999709	-0.494499
C	-12.027752	-6.222374	0.233838
H	-10.411377	-4.840811	-0.239989
H	-11.504666	-5.163452	-1.581499

C	-11.318151	-7.500118	-0.181935
H	-11.927558	-6.093396	1.317600
H	-13.097107	-6.306559	0.022110
H	-11.436826	-7.676753	-1.261672
H	-10.239834	-7.439510	0.029467
O	-11.897175	-8.570247	0.554197
C	-11.416477	-9.832013	0.353352
C	-10.388231	-10.156263	-0.538607
C	-12.024559	-10.840651	1.114095
C	-9.978451	-11.487546	-0.659798
H	-9.906590	-9.391543	-1.136196
C	-11.605898	-12.158937	0.981943
H	-12.820033	-10.562400	1.797894
C	-10.578385	-12.493108	0.093224
H	-9.179403	-11.731125	-1.354887
H	-12.084712	-12.932083	1.576622
H	-10.253224	-13.524032	-0.008134

M1

SCF Done: -1578.701319 .a.u

C	-1.200261	-0.816740	0.393527
H	-1.329113	-0.836714	1.482585
H	-1.107369	0.244476	0.127613
C	-2.380103	-1.457301	-0.334553
C	-3.665281	-0.697578	-0.045773
H	-2.500399	-2.501741	-0.027001
H	-2.195343	-1.463319	-1.412630
H	-3.867240	-0.665056	1.035617
H	-3.589376	0.339251	-0.404139

N	1.245207	-1.040790	0.854798
H	0.983476	-0.771518	1.845775
C	0.111861	-1.483955	0.052765
O	0.271273	-2.305974	-0.818544
C	2.448650	-1.808670	0.640519
C	3.402586	-1.266083	-0.254546
C	2.661132	-3.048779	1.194930
C	4.557884	-2.009826	-0.616107
C	3.826313	-3.783791	0.866806
H	1.921886	-3.468819	1.869215
C	4.057961	0.551548	-1.573215
C	5.459516	-1.407054	-1.530105
C	4.747509	-3.287562	-0.028929
H	3.978948	-4.758567	1.318552
C	5.206803	-0.141873	-2.011376
H	3.837870	1.571148	-1.869794
H	6.348904	-1.951205	-1.835067
H	5.631342	-3.861496	-0.290960
H	5.882574	0.342850	-2.706938
C	-5.985185	-0.871196	-0.606996
C	-6.321633	0.278352	0.117045
C	-6.983994	-1.588309	-1.281557
C	-7.654784	0.698355	0.158708
H	-5.564494	0.848120	0.642275
C	-8.304505	-1.157884	-1.230350
H	-6.696175	-2.475475	-1.836473
C	-8.650732	-0.010123	-0.508720
H	-7.907217	1.592639	0.722092

H	-9.069512	-1.721481	-1.757474
H	-9.682940	0.324451	-0.470561
O	-4.721078	-1.373562	-0.716456
N	3.195611	0.003971	-0.733164
O	2.221144	2.763940	-0.477509
O	0.297800	2.603235	-1.646569
O	0.327066	1.875609	1.468988
O	0.357330	0.222364	3.024236
C	1.550153	4.665756	-1.713891
C	1.286327	3.230898	-1.281355
C	0.046061	1.364658	2.620068
C	-0.757671	2.290240	3.517226
H	-0.147667	3.161819	3.777009
H	-1.061663	1.769354	4.426510
H	-1.635876	2.658849	2.978337
H	1.335046	5.336503	-0.874475
H	2.600586	4.807216	-1.985251
H	0.902771	4.923621	-2.554127
Pd	1.675333	0.958031	0.239348

M2

SCF Done: -1349.597959 .a.u

C	-1.064895	-0.858628	-0.457776
H	-0.971056	-0.046242	0.272609
H	-1.045440	-0.364450	-1.436367
C	-2.380015	-1.609827	-0.260491
C	-3.564085	-0.665305	-0.383569
H	-2.397280	-2.091542	0.722105
H	-2.473209	-2.411112	-1.000174

H	-3.505921	0.135046	0.368967
H	-3.582640	-0.188232	-1.374685
N	1.373759	-1.161129	-0.509312
C	0.145524	-1.772256	-0.340196
O	0.009827	-2.972329	-0.109277
C	2.573528	-1.871294	-0.431497
C	3.748054	-1.088206	-0.633505
C	2.766186	-3.233551	-0.184376
C	5.062397	-1.636141	-0.592212
C	4.068277	-3.778645	-0.142785
H	1.905821	-3.863276	-0.025930
C	4.584109	1.066127	-1.078068
C	6.141346	-0.745260	-0.810564
C	5.204055	-3.020395	-0.338577
H	4.165123	-4.842920	0.052810
C	5.909134	0.593125	-1.051527
H	4.335558	2.105839	-1.261968
H	7.156190	-1.132760	-0.785414
H	6.195314	-3.461213	-0.302196
H	6.723805	1.288194	-1.220760
C	-5.951928	-0.784622	-0.256127
C	-6.107296	0.584987	-0.502920
C	-7.084671	-1.588479	-0.057286
C	-7.392331	1.134630	-0.548023
H	-5.245813	1.223074	-0.659083
C	-8.354976	-1.027017	-0.105228
H	-6.937560	-2.646925	0.132238
C	-8.519463	0.340767	-0.351280

H	-7.503150	2.198611	-0.740181
H	-9.223867	-1.660790	0.050469
H	-9.513033	0.777143	-0.388269
O	-4.752268	-1.426960	-0.190076
N	3.563415	0.243647	-0.875164
O	1.773708	2.887229	-1.283736
O	-0.182818	1.943837	-1.014809
C	-0.166550	4.329412	-1.413554
C	0.498344	2.996610	-1.238634
H	-0.378462	4.755518	-0.425905
H	0.489696	5.013179	-1.955904
H	-1.116457	4.207586	-1.939846
Pd	1.649681	0.823961	-0.892891

M3

SCF Done: -1349.612479 .a.u

C	-1.421732	-2.766672	-0.612662
H	-1.596189	-1.979781	-1.342452
H	-1.410281	-3.726974	-1.138080
C	-2.558087	-2.776915	0.432986
C	-2.522153	-1.557545	1.344601
H	-2.459175	-3.666791	1.064454
H	-3.526394	-2.829976	-0.077245
H	-3.312500	-1.600515	2.105859
H	-1.557061	-1.517319	1.857370
N	0.521629	-1.383904	0.042397
C	-0.100147	-2.613308	0.123138
O	0.291093	-3.527534	0.851824
C	1.467390	-0.976219	0.987262

C	1.858891	0.391717	0.888335
C	2.019913	-1.713045	2.037793
C	2.742916	1.011158	1.814966
C	2.901097	-1.100859	2.956956
H	1.761766	-2.755154	2.137262
C	1.601154	2.392842	-0.315807
C	3.035768	2.382665	1.612376
C	3.265769	0.226576	2.870652
H	3.302852	-1.713337	3.759468
C	2.470713	3.070259	0.560295
H	1.121689	2.878439	-1.157744
H	3.710800	2.883627	2.301038
H	3.945220	0.676577	3.587920
H	2.678103	4.121228	0.392995
C	-2.146341	0.792436	0.900798
C	-1.431727	1.020092	2.083119
C	-2.304539	1.836912	-0.024530
C	-0.864919	2.276537	2.313930
H	-1.302499	0.236609	2.819162
C	-1.747698	3.085101	0.225505
H	-2.860747	1.636921	-0.934034
C	-1.016491	3.313986	1.396168
H	-0.299710	2.436558	3.227892
H	-1.875928	3.879585	-0.504466
H	-0.574792	4.286808	1.589080
O	-2.711467	-0.391715	0.539406
N	1.327895	1.109014	-0.145227
O	-1.081224	-0.653628	-2.986946

O	-0.333516	1.403602	-2.904531
C	-1.664208	0.795485	-4.832419
C	-1.006574	0.502214	-3.515834
H	-1.848533	1.867110	-4.934582
H	-0.998965	0.476210	-5.643212
H	-2.597179	0.233202	-4.918541
Pd	0.131562	0.055448	-1.350347

M4

SCF Done: -1349.603500 .a.u

C	0.575616	3.035140	-1.395852
H	0.279583	3.056982	-2.451987
H	1.018407	4.014783	-1.169783
C	2.275163	2.061613	0.168466
C	1.531716	1.855348	-1.153983
H	3.213345	2.608609	0.025020
H	2.243396	1.739525	-1.979103
N	-1.017962	1.541569	-0.423022
C	-0.700866	2.874106	-0.565389
O	-1.340092	3.818399	-0.107443
C	-2.106200	1.028211	0.264428
C	-2.214204	-0.406375	0.280883
C	-3.071033	1.763060	0.953652
C	-3.260843	-1.052931	1.001886
C	-4.108113	1.109431	1.652079
H	-2.999720	2.841014	0.946336
C	-1.293725	-2.454629	-0.355605
C	-3.269016	-2.470426	1.005265
C	-4.215209	-0.265180	1.691171

H	-4.836600	1.719367	2.179585
C	-2.291107	-3.171931	0.337291
H	-0.501258	-2.962845	-0.896914
H	-4.053950	-2.990220	1.548807
H	-5.012176	-0.754927	2.243005
H	-2.273931	-4.256744	0.333546
N	-1.263657	-1.134056	-0.387383
Pd	0.318584	0.200779	-1.035458
O	1.668344	-1.261675	-1.860172
O	3.728628	-0.745490	-1.069896
C	2.892559	-1.413846	-1.837158
C	3.574456	-2.423496	-2.719259
H	4.316050	-1.918440	-3.346590
H	2.839568	-2.930757	-3.343985
H	4.111805	-3.150139	-2.101215
H	1.669963	2.635737	0.872578
H	3.263958	-0.132822	-0.422916
O	2.709323	0.831977	0.818576
C	1.803140	0.106846	1.582648
C	2.111814	-1.244552	1.771361
C	0.655306	0.649741	2.165795
C	1.245304	-2.060075	2.495922
H	3.020887	-1.646722	1.336373
C	-0.206054	-0.179943	2.884240
H	0.389404	1.688784	2.029901
C	0.073581	-1.536442	3.045085
H	1.488198	-3.111131	2.625218
H	-1.116739	0.243838	3.296167

H	-0.613182	-2.176900	3.589284
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M5

SCF Done: -1042.094525 .a.u

C	-0.734219	-2.920223	-1.559201
H	-0.691313	-3.687084	-2.337985
H	-1.061179	-3.412478	-0.634574
C	-2.656321	-1.339254	-1.078542
C	-1.707921	-1.835969	-1.934077
H	-3.428603	-0.667465	-1.433386
H	-1.724110	-1.528323	-2.978498
N	0.748255	-1.099103	-0.966057
C	0.697987	-2.424722	-1.319709
O	1.655263	-3.184211	-1.406119
C	1.934109	-0.434023	-0.644631
C	1.792019	0.964343	-0.397350
C	3.213597	-0.977799	-0.540162
C	2.902003	1.789026	-0.059353
C	4.312607	-0.159289	-0.196912
H	3.350947	-2.031722	-0.727756
C	0.318206	2.791675	-0.321974
C	2.646027	3.166841	0.147742
C	4.182354	1.192439	0.041346
H	5.291713	-0.623967	-0.123217
C	1.368646	3.667428	0.014398
H	-0.707895	3.116982	-0.451344
H	3.472884	3.822056	0.408344
H	5.039134	1.806812	0.300379
H	1.154940	4.720046	0.163122

N	0.535548	1.499214	-0.509109
Pd	-0.891147	0.094126	-0.944652
O	-2.343332	1.547237	-0.941073
O	-2.977804	0.760514	1.075629
C	-3.061801	1.573526	0.158757
C	-4.024385	2.753611	0.210353
H	-4.767718	2.591690	0.993133
H	-4.513693	2.902242	-0.756329
H	-3.465719	3.669128	0.439801
H	-2.763422	-1.715725	-0.066165

M6-HN-2A

SCF Done: -1216.145952 .a.u

C	1.348654	-3.470222	-0.049418
H	1.529612	-4.342393	-0.685257
H	1.396329	-3.811423	0.992741
C	-0.976629	-2.657367	0.616470
C	-0.012328	-2.890986	-0.336789
H	-2.003711	-2.461458	0.336977
H	-0.292075	-2.811986	-1.386572
N	2.102549	-1.189012	-0.078125
C	2.509108	-2.481640	-0.260472
O	3.642006	-2.880640	-0.514560
C	2.953898	-0.096122	-0.142033
C	2.322786	1.179096	0.033080
C	4.334441	-0.110699	-0.351245
C	3.077377	2.389398	-0.010178
C	5.072603	1.090296	-0.385120
H	4.823737	-1.063582	-0.488608

C	0.329793	2.366735	0.379312
C	2.373553	3.606618	0.154341
C	4.475953	2.322167	-0.220954
H	6.144977	1.030834	-0.549771
C	1.010239	3.598557	0.344569
H	-0.740942	2.304580	0.529809
H	2.926211	4.542004	0.122867
H	5.053183	3.241256	-0.254749
H	0.448136	4.518103	0.466506
N	0.962132	1.209703	0.235728
Pd	0.104011	-0.692410	0.252364
H	-0.789814	-2.891604	1.661735
C	-1.775253	0.008303	0.517466
C	-2.803424	0.071136	-0.493721
C	-2.338521	0.531625	1.656609
C	-3.960902	0.656578	0.103718
C	-2.862369	-0.311790	-1.843868
H	-1.920067	0.658606	2.646691
N	-3.657572	0.930603	1.420729
C	-5.143286	0.869349	-0.613519
C	-4.037979	-0.110596	-2.558046
H	-1.989554	-0.751824	-2.320416
C	-4.547991	1.556055	2.370842
C	-5.166093	0.475718	-1.948102
H	-6.014394	1.323466	-0.149468
H	-4.091286	-0.403125	-3.602948
H	-4.062986	1.581876	3.349297
H	-4.793717	2.584292	2.075207

H	-5.482592	0.989600	2.462158
H	-6.070168	0.625663	-2.531611

M6-2A-OH

SCF Done: -1252.042740 .a.u

C	1.288018	-3.438209	-0.080294
H	1.459490	-4.304910	-0.726146
H	1.325139	-3.793463	0.957609
C	-1.024749	-2.593527	0.586011
C	-0.063028	-2.836144	-0.367416
H	-2.048428	-2.381933	0.305717
H	-0.340254	-2.746526	-1.416975
N	2.077085	-1.167982	-0.084916
C	2.464949	-2.465678	-0.272409
O	3.594090	-2.880440	-0.517882
C	2.946553	-0.088835	-0.135760
C	2.334278	1.195906	0.036150
C	4.328912	-0.125088	-0.330342
C	3.108583	2.394084	0.002368
C	5.086605	1.063857	-0.353552
H	4.804136	-1.085363	-0.465375
C	0.356941	2.415042	0.360640
C	2.422601	3.622308	0.159932
C	4.508059	2.304863	-0.193414
H	6.159580	0.987452	-0.506968
C	1.057228	3.635915	0.333976
H	-0.716331	2.370591	0.498264
H	2.990516	4.548727	0.135415
H	5.100158	3.214701	-0.219625

H	0.508314	4.564235	0.449338
N	0.972213	1.247895	0.224874
Pd	0.084644	-0.640888	0.233778
H	-0.842538	-2.836443	1.630113
C	-1.786951	0.082974	0.492392
C	-2.821990	0.121976	-0.513131
C	-2.334614	0.646646	1.621510
C	-3.971366	0.734513	0.070107
C	-2.878734	-0.313942	-1.846957
H	-1.901199	0.798562	2.601014
N	-3.643737	1.055128	1.374062
C	-5.151171	0.916667	-0.652443
C	-4.057273	-0.138632	-2.562408
H	-2.020646	-0.772748	-2.328360
C	-5.183802	0.472351	-1.970972
H	-6.024626	1.386576	-0.208233
H	-6.091719	0.598778	-2.557614
H	-4.266197	1.471036	2.048018
O	-4.083006	-0.580631	-3.865135
H	-4.954720	-0.384656	-4.240028

M6-N-2A

SCF Done: -1232.188589 .a.u

C	1.407719	-3.493798	0.058802
H	1.600962	-4.383124	-0.548942
H	1.464817	-3.799456	1.111410
C	-0.927651	-2.696015	0.706836
C	0.036684	-2.946712	-0.242146
H	-1.959322	-2.526897	0.426721

H	-0.247233	-2.907129	-1.293048
N	2.122848	-1.202060	-0.043744
C	2.550040	-2.492854	-0.190065
O	3.687621	-2.879961	-0.440153
C	2.955984	-0.097380	-0.146231
C	2.305367	1.171866	-0.004562
C	4.335143	-0.095999	-0.363706
C	3.040019	2.392413	-0.085545
C	5.053609	1.115299	-0.436956
H	4.839391	-1.044349	-0.476000
C	0.296105	2.336993	0.324939
C	2.318015	3.602281	0.051608
C	4.438181	2.341545	-0.303639
H	6.125768	1.068229	-0.606635
C	0.956415	3.577941	0.253062
H	-0.772138	2.263602	0.486463
H	2.855352	4.545113	-0.008524
H	5.000359	3.268366	-0.366453
H	0.380646	4.491230	0.356289
N	0.945483	1.186530	0.205199
Pd	0.118798	-0.727603	0.276986
H	-0.733509	-2.891968	1.758654
C	-1.769019	-0.040380	0.515701
C	-2.760265	0.073827	-0.522776
C	-2.366869	0.455708	1.652592
C	-3.929750	0.658644	0.058250
C	-2.831777	-0.234706	-1.886219
H	-1.976097	0.543601	2.657997

N	-3.668679	0.888168	1.389740
C	-4.019793	0.045900	-2.557515
H	-1.981741	-0.674469	-2.402637
C	-4.600571	1.470307	2.332366
C	-5.097534	0.626766	-1.862946
H	-4.125793	-0.174473	-3.615100
H	-4.812600	0.776562	3.154061
H	-4.206000	2.403786	2.750503
H	-5.525744	1.681911	1.793729
H	-6.024260	0.848229	-2.388689
N	-5.074389	0.942085	-0.562953

M6-HO-2A

SCF Done: -1252.042256 .a.u

C	1.548117	-3.558593	0.526910
H	1.775803	-4.508135	0.032962
H	1.672619	-3.713482	1.606381
C	-0.796013	-2.810312	1.189802
C	0.131372	-3.142341	0.229527
H	-1.847916	-2.737706	0.946205
H	-0.205907	-3.271396	-0.798012
N	2.099557	-1.261024	0.091362
C	2.605456	-2.531448	0.087183
O	3.753127	-2.878522	-0.176695
C	2.852105	-0.133160	-0.205135
C	2.127947	1.103439	-0.195996
C	4.216791	-0.080738	-0.495955
C	2.780140	2.343804	-0.463968
C	4.852014	1.149653	-0.763145

H	4.775717	-1.004533	-0.510360
C	0.070122	2.186055	0.109268
C	1.992307	3.519401	-0.429804
C	4.166794	2.345494	-0.750990
H	5.915977	1.142338	-0.983504
C	0.648232	3.444229	-0.143433
H	-0.982889	2.077219	0.331786
H	2.466324	4.476251	-0.632513
H	4.665499	3.287657	-0.957662
H	0.022781	4.329578	-0.111269
N	0.780225	1.066307	0.079015
Pd	0.079230	-0.870007	0.427988
H	-0.537054	-2.828708	2.245046
C	-1.835974	-0.243444	0.614748
C	-2.644153	0.305355	-0.457982
C	-2.624024	-0.171984	1.728214
C	-3.905474	0.686428	0.085506
C	-2.410794	0.519408	-1.825040
N	-3.897768	0.337487	1.436382
C	-4.902257	1.281137	-0.683995
C	-3.404095	1.113263	-2.600221
H	-1.457993	0.233271	-2.262379
C	-4.634428	1.495180	-2.036652
H	-5.855744	1.569362	-0.248742
H	-3.227082	1.286753	-3.658069
H	-5.390754	1.960241	-2.662344
H	-4.446054	0.833474	2.126699
O	-2.323898	-0.529290	3.011917

H	-3.088596	-0.992234	3.392802
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M7-HN-2A

SCF Done: -1216.163030 .a.u

C	1.003723	-3.215722	0.120944
H	1.131657	-4.158525	-0.426461
H	1.007547	-3.468547	1.190913
C	-1.603752	-2.766170	0.465215
C	-0.283612	-2.485261	-0.239382
H	-2.233302	-3.523782	-0.022924
H	-0.426838	-2.439723	-1.325518
N	1.929739	-0.992418	-0.046042
C	2.242634	-2.333884	-0.124478
O	3.361393	-2.801743	-0.316047
C	2.825923	0.057848	-0.053216
C	2.273561	1.358210	0.235672
C	4.197160	-0.028941	-0.301586
C	3.113059	2.515308	0.245322
C	5.009700	1.121941	-0.277883
H	4.618171	-1.002149	-0.509176
C	0.397168	2.643734	0.750195
C	2.501914	3.763902	0.518486
C	4.497290	2.375421	-0.016536
H	6.071524	1.007349	-0.479135
C	1.149828	3.835404	0.765763
H	-0.670495	2.657073	0.943624
H	3.117932	4.659553	0.526892
H	5.131743	3.256867	-0.010077
H	0.659396	4.780927	0.972883

N	0.929872	1.458598	0.501883
Pd	-0.005225	-0.542013	0.270109
H	-1.434871	-3.095008	1.497494
C	-2.284462	-1.406969	0.461354
C	-3.180236	-0.880284	-0.543025
C	-2.159219	-0.404669	1.428974
C	-3.585842	0.411674	-0.111645
C	-3.672311	-1.389628	-1.752861
H	-1.734316	-0.470967	2.421692
N	-2.964196	0.678987	1.092779
C	-4.462812	1.201239	-0.862758
C	-4.548868	-0.611499	-2.499250
H	-3.368040	-2.372925	-2.099558
C	-3.168019	1.863756	1.897188
C	-4.936642	0.669782	-2.057979
H	-4.768278	2.187728	-0.527858
H	-4.939677	-0.990685	-3.438552
H	-2.444352	1.866834	2.714806
H	-3.018726	2.768052	1.296678
H	-4.180347	1.890098	2.318725
H	-5.622565	1.255074	-2.663360

M7-2A-OH

SCF Done: -1252.059270 .a.u

C	0.994296	-3.197491	0.176042
H	1.103406	-4.159606	-0.340833
H	1.003725	-3.414689	1.253769
C	-1.605305	-2.674522	0.531227
C	-0.285215	-2.459328	-0.198392

H	-2.267882	-3.424727	0.076695
H	-0.439058	-2.450098	-1.283760
N	1.955855	-0.995076	-0.070593
C	2.246348	-2.343516	-0.108044
O	3.355989	-2.834960	-0.292196
C	2.865617	0.042093	-0.112835
C	2.332262	1.356638	0.148431
C	4.233345	-0.067826	-0.370652
C	3.184900	2.503486	0.121734
C	5.059375	1.073713	-0.383973
H	4.640912	-1.051263	-0.556340
C	0.475770	2.675452	0.654099
C	2.590137	3.765086	0.371386
C	4.564667	2.339909	-0.150094
H	6.117834	0.941384	-0.591986
C	1.241711	3.858573	0.632638
H	-0.591110	2.703079	0.859963
H	3.215967	4.653734	0.351766
H	5.210063	3.213115	-0.171988
H	0.765182	4.814592	0.823356
N	0.993088	1.480175	0.426220
Pd	0.031716	-0.507984	0.247658
H	-1.435494	-2.972177	1.572617
C	-2.233720	-1.288955	0.485337
C	-3.096114	-0.759827	-0.551205
C	-2.093221	-0.269413	1.434550
C	-3.464665	0.555714	-0.165261
C	-3.574544	-1.299924	-1.750632

H	-1.677801	-0.327031	2.431180
N	-2.868557	0.817648	1.058230
C	-4.285702	1.346936	-0.968653
C	-4.402516	-0.514725	-2.546507
H	-3.309036	-2.300214	-2.075108
C	-4.750590	0.796921	-2.158918
H	-4.562771	2.356964	-0.681492
H	-5.397622	1.387840	-2.803672
H	-2.901138	1.696990	1.548400
O	-4.860330	-1.063738	-3.715668
H	-5.406513	-0.410469	-4.178468

M7-N-2A

SCF Done: -1232.204543 .a.u

C	1.024257	-3.260427	0.213287
H	1.185834	-4.219324	-0.295944
H	0.986409	-3.476984	1.290454
C	-1.605796	-2.819773	0.424557
C	-0.253407	-2.556361	-0.225227
H	-2.231302	-3.555934	-0.099704
H	-0.343631	-2.540258	-1.318035
N	1.933567	-1.031450	-0.003405
C	2.263861	-2.371194	-0.012169
O	3.394653	-2.832216	-0.135512
C	2.815272	0.031919	-0.016698
C	2.230963	1.335402	0.181144
C	4.197368	-0.044543	-0.196451
C	3.050593	2.506118	0.162803
C	4.991167	1.119877	-0.193316

H	4.641618	-1.019537	-0.336673
C	0.309130	2.615001	0.517458
C	2.406501	3.757424	0.327103
C	4.447981	2.376174	-0.024346
H	6.062976	1.013410	-0.337909
C	1.041684	3.819180	0.494149
H	-0.768876	2.621196	0.643125
H	3.007251	4.663277	0.311907
H	5.068069	3.267694	-0.037312
H	0.525366	4.766355	0.610159
N	0.874805	1.426786	0.379504
Pd	-0.014716	-0.598324	0.237263
H	-1.486141	-3.167204	1.457540
C	-2.259445	-1.444358	0.422253
C	-3.117710	-0.862274	-0.583166
C	-2.154809	-0.479147	1.432670
C	-3.512724	0.420902	-0.109814
C	-3.610706	-1.258509	-1.829356
H	-1.744673	-0.589357	2.427485
N	-2.927749	0.630635	1.122380
C	-4.441453	-0.367207	-2.504024
H	-3.350994	-2.222052	-2.258365
C	-3.144731	1.787459	1.969185
C	-4.747358	0.879953	-1.928988
H	-4.853325	-0.620612	-3.475216
H	-2.190613	2.154716	2.358315
H	-3.617646	2.560619	1.361623
H	-3.803533	1.544017	2.810789

H	-5.391032	1.577414	-2.460334
N	-4.295078	1.294296	-0.739548

M7-HO-2A

SCF Done: -1252.053646 .a.u

C	1.002767	-3.270519	0.241165
H	1.144798	-4.252693	-0.227664
H	1.004366	-3.435059	1.328150
C	-1.605248	-2.762713	0.578840
C	-0.291947	-2.582853	-0.179268
H	-2.296229	-3.491506	0.130471
H	-0.445089	-2.649694	-1.262909
N	1.916335	-1.057226	-0.094946
C	2.239190	-2.398455	-0.064384
O	3.364113	-2.868879	-0.205517
C	2.795969	0.003577	-0.151239
C	2.217929	1.311341	0.046440
C	4.173122	-0.075971	-0.367451
C	3.039007	2.480339	-0.002303
C	4.966667	1.087673	-0.401908
H	4.612655	-1.053639	-0.505049
C	0.312717	2.595072	0.451829
C	2.403049	3.733161	0.182138
C	4.429854	2.346857	-0.230656
H	6.033899	0.978779	-0.576155
C	1.045996	3.798034	0.403790
H	-0.760186	2.601959	0.627467
H	3.004498	4.637913	0.143721
H	5.050685	3.237163	-0.268997

H	0.538015	4.746748	0.543027
N	0.868605	1.406840	0.285288
Pd	-0.023981	-0.614857	0.168120
H	-1.421873	-3.067326	1.614714
C	-2.214144	-1.364747	0.576123
C	-2.977245	-0.722786	-0.490732
C	-2.277755	-0.485983	1.654010
C	-3.469000	0.508284	0.010851
C	-3.283113	-1.094014	-1.804947
N	-3.067223	0.611044	1.348794
C	-4.213548	1.388868	-0.767986
C	-4.038125	-0.224416	-2.588043
H	-2.921548	-2.034874	-2.208358
C	-4.490592	1.005531	-2.080410
H	-4.572954	2.333540	-0.369747
H	-4.276684	-0.496969	-3.611698
H	-5.070262	1.667348	-2.716593
H	-2.973056	1.493880	1.832879
O	-1.789678	-0.664355	2.904771
H	-2.462916	-0.395295	3.552358

M8-HN-2A

SCF Done: -1445.283479 .a.u

C	-0.531731	3.133064	-0.355785
H	-0.620300	3.415718	-1.414041
H	-0.244600	4.044574	0.185489
C	1.131735	1.987718	1.203323
C	0.496248	2.007188	-0.195686
H	1.646507	2.950495	1.366758

H	1.292683	2.097390	-0.942651
N	-2.107739	1.361010	0.010402
C	-1.935666	2.727864	0.091082
O	-2.795409	3.537186	0.426508
C	-3.301044	0.683373	0.214342
C	-3.262583	-0.739864	0.006789
C	-4.520889	1.250188	0.588186
C	-4.433047	-1.539458	0.177106
C	-5.668830	0.447522	0.750901
H	-4.563957	2.317440	0.748083
C	-1.984225	-2.612518	-0.556712
C	-4.305410	-2.933277	-0.045538
C	-5.647171	-0.917620	0.555436
H	-6.596549	0.932634	1.042386
C	-3.091641	-3.472834	-0.409596
H	-1.005416	-2.989462	-0.839819
H	-5.180510	-3.566513	0.076693
H	-6.538906	-1.523323	0.687071
H	-2.973822	-4.537259	-0.583588
N	-2.069750	-1.307734	-0.358886
H	0.343134	1.932710	1.963616
C	2.095696	0.855375	1.391714
C	3.360334	0.680674	0.723092
C	1.908383	-0.272007	2.150321
C	3.883980	-0.582153	1.133191
C	4.099950	1.456656	-0.183921
H	1.074701	-0.538185	2.786201
N	2.979357	-1.143739	2.009764

C	5.109857	-1.067891	0.668647
C	5.320323	0.976467	-0.650776
H	3.725901	2.422068	-0.512808
C	3.104526	-2.448040	2.619416
C	5.820848	-0.272456	-0.227141
H	5.497501	-2.029734	0.991710
H	5.900853	1.572677	-1.348918
H	2.274326	-2.596782	3.312832
H	3.075988	-3.243387	1.864059
H	4.043934	-2.529265	3.178457
H	6.778082	-0.620175	-0.605046
Pd	-0.531675	0.232688	-0.433474
O	1.149391	-1.046031	-0.946192
C	1.821611	-0.780668	-1.947287
O	1.491118	0.191083	-2.788127
H	0.676962	0.622142	-2.418129
C	3.077286	-1.508567	-2.303900
H	3.930504	-0.884111	-2.015520
H	3.128747	-2.446267	-1.751230
H	3.126134	-1.684103	-3.381490

M8-2A-OH

SCF Done: -1481.179627 .a.u

C	-0.386167	2.964688	-0.629763
H	-0.394286	3.114745	-1.718312
H	-0.059350	3.915828	-0.188495
C	1.099727	1.919738	1.160515
C	0.541990	1.799797	-0.266142
H	1.668366	2.863348	1.233039

H	1.380149	1.736587	-0.968623
N	-2.112356	1.368903	-0.148978
C	-1.839770	2.719471	-0.227811
O	-2.651771	3.623089	-0.052225
C	-3.364153	0.807773	0.057151
C	-3.424266	-0.629568	0.029550
C	-4.555876	1.501289	0.276201
C	-4.661039	-1.317323	0.218622
C	-5.769981	0.807919	0.459614
H	-4.525152	2.580615	0.300152
C	-2.264655	-2.643241	-0.212362
C	-4.629232	-2.733635	0.178316
C	-5.843028	-0.569188	0.435665
H	-6.672528	1.389727	0.626634
C	-3.442027	-3.398490	-0.034703
H	-1.303278	-3.120536	-0.380430
H	-5.556344	-3.283561	0.318998
H	-6.785105	-1.089510	0.581159
H	-3.397222	-4.482031	-0.067889
N	-2.260003	-1.321128	-0.182999
H	0.270372	2.010648	1.872498
C	1.977933	0.769921	1.552569
C	3.258377	0.435247	0.981510
C	1.691254	-0.218918	2.460679
C	3.695574	-0.774654	1.597395
C	4.069280	1.045541	0.011308
H	0.816889	-0.337266	3.085658
N	2.713927	-1.150750	2.494932

C	4.915532	-1.364882	1.270641
C	5.287576	0.456004	-0.313033
H	3.778148	1.968021	-0.479480
C	5.706894	-0.740717	0.308114
H	5.248368	-2.283891	1.745052
H	6.665032	-1.177763	0.034360
Pd	-0.605225	0.086787	-0.345229
O	1.000892	-1.353764	-0.579376
C	1.743014	-1.274673	-1.562745
O	1.533321	-0.408947	-2.545322
H	0.737346	0.125564	-2.288338
C	2.957904	-2.128756	-1.734448
H	3.831387	-1.548093	-1.417280
H	2.878650	-3.011121	-1.099340
H	3.089015	-2.408050	-2.782450
H	2.746388	-1.958481	3.095122
O	6.060996	1.080519	-1.262067
H	6.895835	0.596622	-1.351333

M8-N-2A

SCF Done: -1461.325394 .a.u

C	-0.535614	3.131774	-0.387462
H	-0.617123	3.401796	-1.449519
H	-0.253121	4.049982	0.144785
C	1.131743	2.012956	1.190048
C	0.492578	2.008982	-0.208339
H	1.633983	2.983557	1.344747
H	1.288569	2.087521	-0.957709
N	-2.112792	1.363320	-0.008163

C	-1.942518	2.731270	0.053975
O	-2.805581	3.544443	0.370329
C	-3.307565	0.687338	0.197017
C	-3.265163	-0.738918	0.015053
C	-4.531150	1.258949	0.549914
C	-4.435672	-1.537382	0.189227
C	-5.679522	0.457462	0.716536
H	-4.577245	2.328715	0.690982
C	-1.978484	-2.619403	-0.502382
C	-4.303764	-2.934757	-0.006776
C	-5.654058	-0.910787	0.545498
H	-6.610414	0.946214	0.991186
C	-3.085773	-3.478750	-0.349631
H	-0.996516	-3.000025	-0.769041
H	-5.178816	-3.567283	0.119127
H	-6.545994	-1.515498	0.680060
H	-2.964442	-4.545950	-0.502648
N	-2.068043	-1.311237	-0.329495
H	0.347981	1.950897	1.954584
C	2.111428	0.893999	1.374927
C	3.370558	0.733929	0.699050
C	1.933058	-0.251418	2.112715
C	3.895725	-0.540364	1.079985
C	4.142044	1.485069	-0.194446
H	1.099475	-0.530499	2.743099
N	3.000848	-1.121489	1.949223
C	5.349361	0.938415	-0.630208
H	3.815228	2.463067	-0.536763

C	3.138944	-2.441069	2.529642
C	5.751821	-0.330810	-0.173402
H	5.987492	1.483844	-1.318274
H	3.075680	-2.392692	3.621831
H	2.359879	-3.115527	2.155822
H	4.117782	-2.827847	2.242005
H	6.693505	-0.756623	-0.513878
Pd	-0.533523	0.228730	-0.419305
O	1.152472	-1.062915	-0.884947
C	1.832275	-0.827262	-1.888067
O	1.505888	0.117607	-2.760947
H	0.684248	0.553737	-2.414216
C	3.088833	-1.567197	-2.218436
H	3.934063	-0.875949	-2.136213
H	3.232032	-2.387482	-1.516556
H	3.050438	-1.934294	-3.248261
N	5.041214	-1.085804	0.674260

M8-HO-2A

SCF Done: -1481.188340 .a.u

C	-0.383889	3.068965	-0.700450
H	-0.480537	3.259041	-1.778255
H	-0.074015	4.018619	-0.244158
C	1.256758	2.024849	0.951202
C	0.623741	1.942364	-0.447976
H	1.861216	2.944885	1.012570
H	1.427565	1.957143	-1.192463
N	-1.983582	1.362384	-0.153212
C	-1.788753	2.729554	-0.203297

O	-2.632968	3.577945	0.064622
C	-3.189865	0.725571	0.112494
C	-3.179658	-0.709261	0.015655
C	-4.393067	1.343858	0.454313
C	-4.360675	-1.470902	0.264701
C	-5.553563	0.578292	0.693340
H	-4.415218	2.421023	0.529787
C	-1.940908	-2.644366	-0.411678
C	-4.259739	-2.880178	0.154215
C	-5.558237	-0.797929	0.607198
H	-6.468270	1.102380	0.956549
C	-3.060430	-3.469332	-0.180066
H	-0.972592	-3.060302	-0.674920
H	-5.143242	-3.485747	0.339224
H	-6.458446	-1.374378	0.798365
H	-2.962735	-4.546268	-0.266757
N	-2.002214	-1.326325	-0.320552
H	0.462585	2.146565	1.700308
C	2.102917	0.838715	1.299251
C	3.442109	0.543369	0.861457
C	1.686876	-0.273193	1.992929
C	3.791489	-0.746794	1.367256
C	4.375817	1.228550	0.068936
N	2.695699	-1.210791	2.076151
C	5.027794	-1.336754	1.117006
C	5.608606	0.634811	-0.197557
H	4.137363	2.208960	-0.334450
C	5.933247	-0.633114	0.320698

H	5.276331	-2.316323	1.516681
H	6.334578	1.160254	-0.811626
H	6.902510	-1.071007	0.101110
Pd	-0.441837	0.174865	-0.548121
O	1.220383	-1.166031	-0.932448
C	2.006818	-0.966984	-1.862997
O	1.785282	-0.046557	-2.794228
H	0.951761	0.421175	-2.543576
C	3.286852	-1.719670	-2.029146
H	4.109607	-1.082268	-1.683943
H	3.265915	-2.620664	-1.417042
H	3.455718	-1.961609	-3.081513
H	2.572651	-2.131859	2.466093
O	0.492889	-0.584347	2.547487
H	-0.197708	-0.120858	2.036533

M9-HN-2A

SCF Done: -1445.305828 .a.u

C	1.654488	2.669143	-1.142351
H	2.433142	2.090912	-1.649230
H	1.679860	3.690091	-1.534258
C	0.867704	3.275478	1.268591
C	1.973976	2.693922	0.366324
H	1.315756	3.511194	2.244545
H	2.888050	3.287738	0.491862
N	0.049716	0.791896	-1.375463
C	0.278180	2.145088	-1.525365
O	-0.575766	2.930326	-1.943314
C	-1.219929	0.241548	-1.543732

C	-1.373840	-1.082549	-1.034900
C	-2.347811	0.820127	-2.133845
C	-2.605635	-1.793062	-1.083144
C	-3.564580	0.107744	-2.205098
H	-2.274268	1.820579	-2.527883
C	-0.302436	-2.863923	0.059915
C	-2.626099	-3.090308	-0.512686
C	-3.717959	-1.165576	-1.693278
H	-4.410978	0.595411	-2.681439
C	-1.490508	-3.620339	0.059987
H	0.624828	-3.228078	0.486797
H	-3.551500	-3.659740	-0.533727
H	-4.665237	-1.692574	-1.755033
H	-1.489614	-4.607681	0.508023
N	-0.266702	-1.656002	-0.479353
Pd	1.390789	-0.550741	-0.632071
O	2.921353	-1.839738	0.043937
O	3.431362	0.138972	-0.746631
C	3.813048	-0.970059	-0.249483
C	5.270087	-1.261736	-0.038365
H	5.701095	-1.627089	-0.977869
H	5.396579	-2.031399	0.726015
H	5.798286	-0.347497	0.243257
H	0.514053	4.226910	0.852111
H	2.222218	1.685434	0.704390
C	-0.278477	1.031472	2.043577
C	-1.605155	0.513227	1.957190
C	-1.940465	-0.763765	2.416025

C	-0.923044	-1.539677	2.964420
C	0.395645	-1.052475	3.057246
C	0.723480	0.221656	2.603907
C	-0.301141	2.353149	1.463105
C	-1.596028	2.572505	1.067011
H	-2.955462	-1.142125	2.342315
H	-1.151711	-2.537711	3.327664
H	1.168175	-1.682513	3.488715
H	1.743216	0.585289	2.688517
H	-2.013644	3.418524	0.540265
C	-3.811345	1.365829	1.109937
H	-4.389497	1.455649	2.038682
H	-4.112624	2.161202	0.425601
H	-4.040138	0.408086	0.635035
N	-2.390932	1.474461	1.356104

M9-2A-OH

SCF Done: -1481.202916 .a.u

C	-0.890401	3.076322	1.094623
H	-1.472459	2.550053	1.856857
H	-0.783909	4.118969	1.406463
C	-0.836771	3.221553	-1.531110
C	-1.667960	3.019900	-0.244693
H	-1.536380	3.452477	-2.347151
H	-2.443576	3.794061	-0.201108
N	0.730011	1.190291	1.125407
C	0.535288	2.555559	1.034223
O	1.457179	3.362330	0.890226
C	1.984612	0.626507	0.902843

C	1.996515	-0.795694	0.772538
C	3.218831	1.272495	0.761110
C	3.170994	-1.538677	0.462597
C	4.384176	0.538461	0.453405
H	3.260367	2.343837	0.865189
C	0.683381	-2.746100	0.794769
C	3.033904	-2.943697	0.335861
C	4.385355	-0.833234	0.289122
H	5.314810	1.088473	0.341497
C	1.804878	-3.545431	0.502950
H	-0.314410	-3.152091	0.915351
H	3.913280	-3.538708	0.104181
H	5.294227	-1.376929	0.050305
H	1.682169	-4.618622	0.408297
N	0.800852	-1.433501	0.923626
Pd	-0.757265	-0.216868	1.173870
O	-2.345428	-1.581340	1.184225
O	-2.779960	0.558184	1.351388
C	-3.208024	-0.631673	1.211600
C	-4.661707	-0.928401	1.008857
H	-4.948004	-1.821845	1.570695
H	-4.809479	-1.134241	-0.057665
H	-5.274232	-0.075384	1.306461
H	-0.183526	4.095092	-1.421543
H	-2.194567	2.067710	-0.299593
C	-0.476996	0.667467	-2.067560
C	0.667694	-0.153347	-2.285139
C	0.566430	-1.538212	-2.402894

C	-0.697760	-2.114727	-2.296898
C	-1.840881	-1.314886	-2.098081
C	-1.745069	0.067678	-2.000868
C	-0.006340	2.022791	-1.895618
C	1.358264	1.973508	-2.031154
H	1.445108	-2.159779	-2.548619
H	-0.806598	-3.194365	-2.376099
H	-2.647607	0.647688	-1.848081
H	2.080599	2.766574	-1.907222
N	1.773540	0.680922	-2.309584
H	2.725485	0.366090	-2.197257
O	-3.099619	-1.868086	-1.993865
H	-3.005794	-2.824839	-1.873795

M9-N-2A

SCF Done: -1461.347924 .a.u

C	1.701264	2.690278	-1.066184
H	2.459392	2.104506	-1.594144
H	1.753276	3.721229	-1.427828
C	0.917225	3.207785	1.365459
C	2.026524	2.664269	0.442006
H	1.369202	3.441131	2.340040
H	2.937032	3.258800	0.586761
N	0.047821	0.867199	-1.373658
C	0.304803	2.220551	-1.445521
O	-0.542255	3.050375	-1.784897
C	-1.241293	0.360649	-1.548977
C	-1.434304	-0.969762	-1.074079
C	-2.349693	0.988448	-2.123405

C	-2.689747	-1.635716	-1.125999
C	-3.590159	0.317165	-2.206123
H	-2.246193	1.994816	-2.495272
C	-0.412175	-2.818073	-0.043713
C	-2.750513	-2.943236	-0.583859
C	-3.783309	-0.958279	-1.715667
H	-4.421179	0.841152	-2.670828
C	-1.626269	-3.530493	-0.045643
H	0.508125	-3.227806	0.356309
H	-3.697039	-3.476448	-0.601292
H	-4.749214	-1.449971	-1.777201
H	-1.655769	-4.528258	0.377419
N	-0.341420	-1.594362	-0.544811
Pd	1.350869	-0.539584	-0.686351
O	2.848586	-1.890474	-0.054861
O	3.407833	0.097121	-0.788034
C	3.762112	-1.037431	-0.328945
C	5.212005	-1.376167	-0.140611
H	5.621829	-1.732441	-1.093000
H	5.323819	-2.167142	0.604086
H	5.770190	-0.484731	0.155754
H	0.534089	4.154511	0.965596
H	2.281410	1.645242	0.742725
C	-0.160042	0.919293	2.102219
C	-1.479648	0.373143	2.034126
C	-0.879896	-1.613619	2.899772
C	0.458363	-1.201732	3.023624
C	0.832287	0.080109	2.621414

C	-0.225596	2.253091	1.560857
C	-1.538334	2.451019	1.206851
H	-1.170753	-2.615484	3.209653
H	1.194041	-1.889046	3.429022
H	1.863045	0.410238	2.710522
H	-1.985563	3.302323	0.714220
C	-3.729965	1.185258	1.280220
H	-4.298528	1.780498	2.004563
H	-3.992104	1.494529	0.265787
H	-3.978647	0.131201	1.408674
N	-2.304234	1.330165	1.488121
N	-1.861536	-0.846350	2.409779

M9-HO-2A

SCF Done: -1481.217649 .a.u

C	1.433703	2.842029	-0.748593
H	2.258167	2.386922	-1.303163
H	1.399985	3.907918	-0.990583
C	0.489321	2.981998	1.675456
C	1.694046	2.667828	0.764621
H	0.869459	3.137343	2.695139
H	2.532032	3.324848	1.028165
N	-0.025892	0.936998	-1.345230
C	0.099209	2.290408	-1.208578
O	-0.836326	3.089095	-1.419404
C	-1.282649	0.339569	-1.518601
C	-1.358100	-1.026161	-1.122593
C	-2.452961	0.923517	-2.002114
C	-2.566207	-1.773435	-1.163524

C	-3.657239	0.185795	-2.044854
H	-2.438090	1.952286	-2.322327
C	-0.171552	-2.852876	-0.243539
C	-2.510881	-3.121068	-0.727056
C	-3.737197	-1.127923	-1.629879
H	-4.547026	0.684191	-2.418807
C	-1.328111	-3.657052	-0.269097
H	0.785323	-3.215089	0.113792
H	-3.416229	-3.721362	-0.754795
H	-4.672480	-1.677968	-1.669623
H	-1.267316	-4.681278	0.080769
N	-0.204592	-1.600229	-0.667694
Pd	1.395277	-0.405933	-0.755734
O	3.002191	-1.662145	-0.228673
O	3.378898	0.414255	-0.812498
C	3.836552	-0.713217	-0.432285
C	5.309782	-0.930276	-0.253806
H	5.759024	-1.152774	-1.228758
H	5.490771	-1.773688	0.415776
H	5.777273	-0.021985	0.134404
H	0.030322	3.930766	1.371466
H	2.034481	1.646645	0.956396
C	-0.410012	0.555898	2.180337
C	-1.672873	-0.096842	2.041602
C	-1.868797	-1.427449	2.400741
C	-0.773194	-2.135957	2.895913
C	0.481276	-1.518063	3.039915
C	0.669310	-0.180998	2.693611

C	-0.561409	1.909041	1.701381
C	-1.867056	2.012131	1.271778
H	-2.839114	-1.902163	2.286153
H	-0.894860	-3.178598	3.175925
H	1.316992	-2.091056	3.431817
H	1.642373	0.284034	2.821247
N	-2.552745	0.830055	1.511513
H	-3.440542	0.625931	1.077643
O	-2.528611	3.017284	0.669962
H	-1.979652	3.290920	-0.107098

M10-HN-2A

SCF Done: -1445.282564 .a.u

C	0.556877	-0.327628	-0.004069
H	0.432910	0.331030	-0.871928
H	0.429979	0.325860	0.867283
C	1.949965	-0.952185	-0.003754
C	3.052175	0.110788	0.000876
H	2.058568	-1.600142	-0.880909
H	2.055992	-1.605032	0.870111
H	2.923326	0.769657	-0.871461
H	2.920756	0.764718	0.876546
N	-1.842085	-0.877034	-0.005825
C	-0.549323	-1.370308	-0.009155
O	-0.285220	-2.572074	-0.015513
C	-2.957721	-1.715461	-0.006314
C	-4.215249	-1.042087	0.002355
C	-2.999350	-3.113117	-0.013687
C	-5.463654	-1.728493	0.004220

C	-4.235684	-3.795135	-0.012143
H	-2.072393	-3.663038	-0.020348
C	-5.286968	1.052810	0.018498
C	-6.637161	-0.935739	0.013816
C	-5.451396	-3.142737	-0.003399
H	-4.214142	-4.881411	-0.018089
C	-6.554377	0.441290	0.021044
H	-5.154243	2.129355	0.023727
H	-7.605005	-1.429737	0.015494
H	-6.389811	-3.688326	-0.002231
H	-7.442992	1.062425	0.028588
N	-4.179184	0.323373	0.009353
O	-2.691464	3.176625	0.010833
O	-0.638094	2.419230	-0.002297
C	-0.914973	4.821280	-0.041043
C	-1.432336	3.414240	-0.000174
H	-0.707337	5.095445	-1.082040
H	-1.660025	5.511834	0.359682
H	0.019636	4.892671	0.520496
Pd	-2.337272	1.102745	0.002933
C	4.444249	-0.450754	0.001324
C	5.667472	0.313569	0.004455
C	4.820999	-1.770903	-0.001024
C	6.747104	-0.614899	0.003777
C	5.954120	1.687362	0.007710
H	4.211667	-2.663840	-0.003693
N	6.205681	-1.884613	0.000439
C	8.083844	-0.204438	0.006270

C	7.281904	2.100901	0.010188
H	5.148188	2.416567	0.008260
C	6.961809	-3.115694	-0.001167
C	8.335267	1.164452	0.009483
H	8.897791	-0.923782	0.005749
H	7.515108	3.162048	0.012717
H	7.599999	-3.185927	-0.890652
H	7.597516	-3.189808	0.889782
H	6.267953	-3.958995	-0.003975
H	9.362859	1.517147	0.011490

M10-2A-OH

SCF Done: -1481.179687 .a.u

C	0.486499	-0.600110	-0.002497
H	0.427322	0.067366	-0.870406
H	0.424879	0.062997	0.868600
C	1.812247	-1.357180	-0.002714
C	3.011002	-0.404576	0.000658
H	1.856954	-2.012932	-0.879724
H	1.855092	-2.016768	0.871528
H	2.945511	0.263453	-0.871762
H	2.943761	0.259500	0.875961
N	-1.954601	-0.910383	-0.004226
C	-0.716746	-1.528885	-0.006615
O	-0.572341	-2.750842	-0.011543
C	-3.147534	-1.634364	-0.004854
C	-4.332486	-0.840033	0.001894
C	-3.326953	-3.021124	-0.010875
C	-5.642516	-1.399964	0.003080

C	-4.624545	-3.577760	-0.009955
H	-2.458768	-3.659845	-0.016039
C	-5.192324	1.350319	0.014842
C	-6.732122	-0.495315	0.010621
C	-5.769929	-2.808509	-0.003147
H	-4.710354	-4.660869	-0.014802
C	-6.513894	0.866812	0.016573
H	-4.954212	2.408573	0.019177
H	-7.743975	-0.891453	0.011738
H	-6.757637	-3.258769	-0.002439
H	-7.336895	1.572608	0.022522
N	-4.161843	0.515235	0.007642
O	-2.396961	3.207757	0.009866
O	-0.430246	2.248031	-0.000161
C	-0.463431	4.665479	-0.039046
C	-1.120299	3.318023	0.000670
H	-0.211077	4.909459	-1.077645
H	-1.141352	5.430415	0.345328
H	0.464399	4.646167	0.537868
Pd	-2.251618	1.108783	0.003087
C	4.343778	-1.094353	0.000403
C	5.630066	-0.441689	0.002445
C	4.596577	-2.444887	-0.001751
C	6.624693	-1.459587	0.001415
C	6.019745	0.906080	0.005026
H	3.904771	-3.274885	-0.003700
N	5.962601	-2.673952	-0.001150
C	7.985688	-1.154686	0.002912

C	7.376715	1.208223	0.006505
H	5.293071	1.711990	0.005881
C	8.351471	0.188197	0.005460
H	8.743700	-1.933139	0.002128
H	9.405931	0.457722	0.006658
H	6.400411	-3.580451	-0.002445
O	7.732755	2.537761	0.008998
H	8.699924	2.596207	0.010136

M10-N-2A

SCF Done: -1461.325130 .a.u

C	0.557896	-0.310335	-0.003564
H	0.430646	0.347573	-0.871484
H	0.427703	0.342285	0.867918
C	1.953708	-0.928775	-0.003261
C	3.050608	0.139600	0.001320
H	2.065166	-1.576194	-0.880372
H	2.062637	-1.581056	0.870587
H	2.919026	0.797559	-0.871198
H	2.916588	0.792590	0.877200
N	-1.837443	-0.874026	-0.005637
C	-0.542430	-1.359632	-0.008744
O	-0.270075	-2.559584	-0.014997
C	-2.948364	-1.719222	-0.006375
C	-4.209552	-1.053080	0.002054
C	-2.981567	-3.116938	-0.013812
C	-5.453910	-1.746709	0.003606
C	-4.213932	-3.806279	-0.012586
H	-2.051449	-3.661525	-0.020277

C	-5.293471	1.035572	0.018081
C	-6.632028	-0.960850	0.012990
C	-5.433319	-3.160896	-0.004088
H	-4.186044	-4.892383	-0.018582
C	-6.557263	0.416655	0.020316
H	-5.167118	2.112880	0.023400
H	-7.596976	-1.460455	0.014429
H	-6.368526	-3.711946	-0.003158
H	-7.449470	1.032605	0.027706
N	-4.181427	0.312609	0.009133
O	-2.711291	3.174070	0.011212
O	-0.652785	2.430504	-0.001563
C	-0.946715	4.830889	-0.040616
C	-1.453908	3.420119	0.000435
H	-0.753674	5.110937	-1.082869
H	-1.692200	5.514491	0.371158
H	-0.006475	4.907020	0.510717
Pd	-2.344262	1.102738	0.003173
C	4.445618	-0.415449	0.001648
C	5.665981	0.347577	0.004316
C	4.828975	-1.736443	-0.000459
C	6.747655	-0.582326	0.003658
C	6.006841	1.704098	0.007159
H	4.217827	-2.628075	-0.002803
N	6.212156	-1.851690	0.000737
C	7.361313	2.031834	0.009102
H	5.243118	2.477490	0.007817
C	6.980063	-3.079342	-0.000821

C	8.330650	1.012252	0.008180
H	7.680788	3.069292	0.011337
H	8.036280	-2.805452	0.000853
H	6.761509	-3.679562	0.889647
H	6.763443	-3.676106	-0.894081
H	9.387951	1.269974	0.009709
N	8.048343	-0.295713	0.005474

M10-HO-2A

SCF Done: -1481.183098 .a.u

C	0.638747	-0.337130	-0.003243
H	0.538214	0.323442	-0.871920
H	0.535582	0.318614	0.868793
C	2.008018	-1.010794	-0.003213
C	3.162346	-0.003884	0.001433
H	2.072257	-1.654803	-0.890015
H	2.069711	-1.659990	0.880011
H	3.055111	0.658987	-0.870927
H	3.052858	0.653472	0.877679
N	-1.770345	-0.841409	-0.005135
C	-0.490698	-1.356903	-0.007885
O	-0.241778	-2.563512	-0.013441
C	-2.902538	-1.659697	-0.005536
C	-4.146329	-0.962204	0.002492
C	-2.969001	-3.055609	-0.012322
C	-5.406942	-1.625414	0.004311
C	-4.217824	-3.715220	-0.010834
H	-2.052434	-3.622793	-0.018473
C	-5.179332	1.151853	0.017399

C	-6.565868	-0.811523	0.013235
C	-5.420613	-3.039862	-0.002699
H	-4.216479	-4.801618	-0.016318
C	-6.457771	0.563747	0.019871
H	-5.027326	2.225866	0.022178
H	-7.542565	-1.287685	0.014873
H	-6.369026	-3.567830	-0.001545
H	-7.334742	1.201160	0.026902
N	-4.084909	0.402547	0.008887
O	-2.538077	3.227216	0.009910
O	-0.503170	2.422968	-0.002137
C	-0.724006	4.831037	-0.041216
C	-1.274116	3.437040	-0.000558
H	-0.493469	5.093799	-1.080340
H	-1.458729	5.540927	0.344266
H	0.203514	4.883923	0.534057
Pd	-2.228432	1.147761	0.002766
C	4.538965	-0.608460	0.001273
C	5.766414	0.154218	0.004813
C	4.931833	-1.929996	-0.002072
C	6.857180	-0.759951	0.003421
C	6.041359	1.529145	0.009023
N	6.309013	-2.031536	-0.000828
C	8.185175	-0.340529	0.006104
C	7.367731	1.955900	0.011717
H	5.229605	2.251781	0.010147
C	8.428402	1.033260	0.010290
H	9.003057	-1.056194	0.004996

H	7.588296	3.019877	0.014989
H	9.453401	1.392768	0.012473
O	4.268010	-3.112243	-0.006189
H	3.314387	-2.938249	-0.006914
H	6.803667	-2.909227	-0.002583

2a-HN-2A

SCF Done: -1090.614416 .a.u

C	-0.354452	-2.713264	-1.179253
H	-0.031212	-2.243454	-2.119845
H	0.122063	-2.143763	-0.370867
C	1.606372	-4.325755	-1.348482
H	1.895633	-3.851793	-2.299364
C	-1.872494	-2.581188	-1.101928
O	-2.629029	-3.434230	-1.549512
C	-3.603507	-0.956789	-0.333654
C	-3.714801	0.323230	0.306006
C	-4.749943	-1.630377	-0.719552
C	-5.006191	0.884631	0.535581
C	-6.019555	-1.055149	-0.482909
H	-4.657734	-2.593810	-1.199733
C	-2.650667	2.128122	1.258157
C	-5.049659	2.150410	1.171009
C	-6.160635	0.170001	0.128040
H	-6.901270	-1.606452	-0.796852
C	-3.878396	2.774434	1.533281
H	-1.711315	2.603314	1.535776
H	-6.014206	2.613148	1.364298
H	-7.142297	0.600543	0.304500

H	-3.881430	3.743872	2.021191
N	-2.562677	0.951175	0.669266
C	2.082218	-5.749032	-1.331045
C	3.455045	-6.183791	-1.404758
C	1.324473	-6.890898	-1.249248
C	3.450026	-7.606509	-1.361924
C	4.683274	-5.512151	-1.502010
H	2.134506	-3.756445	-0.568419
H	0.251955	-7.006914	-1.178650
C	4.627704	-8.358313	-1.412328
C	5.857175	-6.255050	-1.552629
H	4.715349	-4.426320	-1.537585
C	5.829033	-7.663222	-1.508282
H	4.609187	-9.443794	-1.378175
H	6.813583	-5.745347	-1.627949
H	6.762717	-8.216992	-1.549750
C	1.692166	-9.390697	-1.193491
H	2.098587	-9.889416	-0.305177
H	0.601957	-9.409645	-1.135165
H	2.003959	-9.952678	-2.082095
N	2.135533	-8.017177	-1.267349
C	0.096166	-4.173595	-1.152784
H	-0.445915	-4.716061	-1.933828
H	-0.199405	-4.627706	-0.198513
N	-2.298179	-1.416686	-0.510477
H	-1.607705	-0.760915	-0.156164

2a-2A-OH

SCF Done: -1126.511991 .a.u

C	-0.773301	-3.405096	0.517333
H	-0.123610	-2.525792	0.613128
H	-0.860920	-3.843293	1.521559
C	1.203573	-4.954897	0.071745
H	1.900247	-4.112883	0.180279
C	-2.177258	-3.007813	0.077342
O	-3.000165	-3.836635	-0.291124
C	-3.610833	-0.979854	-0.154283
C	-3.559063	0.442443	0.031483
C	-4.781845	-1.569018	-0.600399
C	-4.715943	1.230306	-0.245939
C	-5.916251	-0.769217	-0.868717
H	-4.811955	-2.640173	-0.738434
C	-2.327651	2.287356	0.645513
C	-4.601837	2.628011	-0.043280
C	-5.899621	0.596720	-0.700777
H	-6.820864	-1.259255	-1.217230
C	-3.413514	3.160097	0.400957
H	-1.377727	2.686165	0.997642
H	-5.460684	3.263897	-0.243076
H	-6.778407	1.199883	-0.910890
H	-3.297466	4.226660	0.565003
N	-2.388429	0.981402	0.470821
C	1.803686	-5.990669	-0.829724
C	1.328998	-7.340381	-1.015908
C	2.881783	-5.840375	-1.666891
C	2.171873	-7.954729	-1.983561
C	0.279055	-8.077129	-0.446949

H	1.069601	-5.373098	1.080335
H	3.514869	-4.977075	-1.821255
C	1.984871	-9.276617	-2.386892
C	0.095065	-9.394734	-0.848761
H	-0.389555	-7.647660	0.291748
C	0.939115	-9.989657	-1.810476
H	2.630102	-9.743088	-3.126142
H	0.767391	-11.023330	-2.104121
N	3.109628	-7.011699	-2.366204
C	-0.153535	-4.435223	-0.432098
H	-0.022899	-3.991880	-1.427218
H	-0.856445	-5.264690	-0.553907
N	-2.428866	-1.658320	0.143447
H	-1.693167	-1.032230	0.456525
O	-0.938328	-10.095187	-0.272697
H	-0.959670	-10.984805	-0.655811
H	3.854479	-7.161633	-3.026930

2a-N-2A

SCF Done: -1106.657769 .a.u

C	-0.759198	-3.374959	0.599839
H	-0.112178	-2.491850	0.673145
H	-0.826651	-3.802875	1.609909
C	1.190507	-4.961648	0.155623
H	1.903072	-4.134723	0.274761
C	-2.174511	-2.993936	0.181336
O	-3.004639	-3.839381	-0.130500
C	-3.615141	-0.978107	-0.101283
C	-3.558843	0.450386	0.024260

C	-4.795693	-1.584539	-0.495340
C	-4.721765	1.227065	-0.258653
C	-5.936217	-0.795584	-0.770330
H	-4.828921	-2.660443	-0.588310
C	-2.313356	2.317680	0.532606
C	-4.603019	2.631875	-0.116762
C	-5.915570	0.576054	-0.659372
H	-6.848577	-1.298690	-1.077461
C	-3.404634	3.180579	0.277386
H	-1.355512	2.729826	0.845642
H	-5.466147	3.259869	-0.322808
H	-6.799015	1.170733	-0.873973
H	-3.284680	4.252874	0.394291
N	-2.378190	1.005635	0.413649
C	1.777407	-5.998752	-0.753371
C	1.249541	-7.311116	-1.020934
C	2.908812	-5.882905	-1.525452
C	2.121000	-7.929760	-1.964785
C	0.154578	-8.069020	-0.590753
H	1.042841	-5.385043	1.160308
H	3.594145	-5.049874	-1.611450
C	0.008715	-9.350652	-1.115176
H	-0.560349	-7.674069	0.125891
C	0.944272	-9.841093	-2.044259
H	0.827316	-10.842317	-2.453872
N	3.129410	-7.036965	-2.260160
C	-0.154379	-4.413733	-0.350163
H	-0.014283	-3.971708	-1.344507

H	-0.874229	-5.228494	-0.473341
N	-2.425635	-1.644206	0.197078
H	-1.683393	-1.004974	0.465350
C	4.221152	-7.289293	-3.177882
H	5.186597	-7.237692	-2.662199
H	4.083268	-8.293119	-3.582342
H	4.216286	-6.565170	-4.000150
N	2.004152	-9.151732	-2.481029
H	-0.824039	-9.979220	-0.816265

2a-HO-2A

SCF Done: -1126.510367 .a.u

C	-0.788429	-3.431651	0.641364
H	-0.140354	-2.553018	0.749868
H	-0.863249	-3.897014	1.633874
C	1.175926	-4.981821	0.144670
H	1.880710	-4.152062	0.278766
C	-2.199937	-3.035829	0.227103
O	-3.045334	-3.872897	-0.065454
C	-3.608254	-1.002786	-0.094063
C	-3.529871	0.427188	0.001047
C	-4.798921	-1.598662	-0.474265
C	-4.680924	1.215780	-0.297556
C	-5.927183	-0.797996	-0.765041
H	-4.848727	-2.675659	-0.544290
C	-2.254992	2.285431	0.468368
C	-4.540127	2.621264	-0.185835
C	-5.885216	0.575256	-0.683387
H	-6.847625	-1.293270	-1.060708

C	-3.332950	3.159624	0.195527
H	-1.290429	2.689104	0.771737
H	-5.393665	3.258033	-0.404664
H	-6.759515	1.179003	-0.909915
H	-3.196220	4.232215	0.289265
N	-2.340474	0.972372	0.377675
C	1.771256	-5.981805	-0.796034
C	1.309778	-7.328815	-1.052541
C	2.864935	-5.804090	-1.597853
C	2.184259	-7.910241	-2.011052
C	0.251514	-8.097723	-0.548081
H	1.035991	-5.439689	1.135117
C	2.013695	-9.209304	-2.484925
C	0.076189	-9.396102	-1.017433
H	-0.427027	-7.682375	0.191739
C	0.943189	-9.944452	-1.979187
H	2.690092	-9.634954	-3.221284
H	0.779426	-10.958385	-2.332474
N	3.163906	-6.966389	-2.305642
C	-0.176509	-4.435244	-0.342479
H	-0.041283	-3.959986	-1.321919
H	-0.886781	-5.254761	-0.489215
N	-2.429822	-1.681368	0.217430
H	-1.675903	-1.049522	0.469587
H	3.695737	-6.954668	-3.164126
H	-0.745728	-9.996562	-0.638195
O	3.619031	-4.681426	-1.771119
H	4.543282	-4.883325	-1.548052

TS1

SCF Done: -1578.696228 .a.u

C	-1.095899	-0.857548	0.396574
H	-1.232044	-0.693521	1.472763
H	-0.982309	0.139674	-0.049614
C	-2.301036	-1.579421	-0.202287
C	-3.555548	-0.731469	-0.066472
H	-2.456386	-2.543496	0.293350
H	-2.119938	-1.794802	-1.259469
H	-3.751009	-0.485499	0.988512
H	-3.443442	0.214626	-0.615014
N	1.350731	-1.037867	0.820872
H	1.093140	-0.642814	2.026861
C	0.197771	-1.624773	0.193470
O	0.271284	-2.655949	-0.443398
C	2.574196	-1.715773	0.499100
C	3.425677	-1.088746	-0.445077
C	2.922790	-2.953765	0.992602
C	4.609199	-1.726121	-0.907228
C	4.112803	-3.587442	0.560542
H	2.266053	-3.449200	1.699137
C	3.827436	0.800414	-1.775339
C	5.389915	-1.030816	-1.865164
C	4.936650	-2.999147	-0.374320
H	4.366262	-4.561386	0.967261
C	4.998745	0.215955	-2.301990
H	3.496556	1.799344	-2.037669
H	6.298558	-1.491236	-2.243037

H	5.841893	-3.495811	-0.710458
H	5.581595	0.767085	-3.031401
C	-5.884928	-0.920647	-0.583077
C	-6.170746	0.362432	-0.101731
C	-6.918027	-1.719065	-1.095785
C	-7.487111	0.832720	-0.138528
H	-5.386581	0.996628	0.294009
C	-8.221256	-1.237099	-1.125242
H	-6.669647	-2.709638	-1.463156
C	-8.516625	0.043935	-0.645872
H	-7.699698	1.830629	0.235596
H	-9.012785	-1.865120	-1.525134
H	-9.535469	0.418498	-0.670217
O	-4.642142	-1.482175	-0.596264
N	3.079193	0.165265	-0.888416
O	1.893130	2.828875	-0.500717
O	-0.215270	2.555180	-1.248753
O	0.388847	1.719273	1.764224
O	0.718068	-0.113303	3.049671
C	0.875048	4.685373	-1.562875
C	0.792620	3.241846	-1.092042
C	0.308980	1.087752	2.853663
C	-0.345921	1.775792	4.026427
H	-0.553221	2.820145	3.792174
H	0.305409	1.702700	4.902344
H	-1.280272	1.258404	4.269866
H	0.848251	5.350562	-0.692513
H	1.818217	4.870101	-2.086108

H	0.029986	4.911597	-2.215622
Pd	1.587123	0.963026	0.228177

TS2

SCF Done: -1349.563255 .a.u

C	-1.066916	-3.283793	-0.619224
H	-0.710422	-3.885208	-1.465463
H	-1.759652	-3.924221	-0.059184
C	-1.786132	-2.037091	-1.155779
C	-2.510254	-1.253611	-0.060477
H	-2.558304	-2.416223	-1.840772
H	-1.569766	-1.358357	-2.386758
H	-3.418498	-1.783204	0.264835
H	-1.860685	-1.128217	0.812453
N	0.753881	-1.827405	-0.012925
C	0.139448	-3.020085	0.276330
O	0.514756	-3.822221	1.127160
C	1.925087	-1.361563	0.573261
C	2.394398	-0.113260	0.059755
C	2.673209	-1.970180	1.579633
C	3.578366	0.505599	0.550012
C	3.849942	-1.354671	2.060434
H	2.336167	-2.915295	1.979268
C	2.009070	1.640337	-1.452916
C	3.942745	1.748045	-0.025998
C	4.308115	-0.147606	1.573139
H	4.406187	-1.858909	2.845677
C	3.167305	2.313547	-1.015765
H	1.356510	2.034116	-2.224253

H	4.840792	2.248444	0.326331
H	5.213098	0.310873	1.959752
H	3.429735	3.265276	-1.464489
C	-2.824663	1.105019	0.258474
C	-3.124170	1.026029	1.622545
C	-2.473668	2.333168	-0.315324
C	-3.070808	2.181678	2.405452
H	-3.407944	0.078386	2.067786
C	-2.433275	3.477937	0.475664
H	-2.210195	2.355572	-1.367007
C	-2.729822	3.409953	1.840434
H	-3.305143	2.115475	3.464378
H	-2.156440	4.427724	0.025806
H	-2.692074	4.304171	2.455263
O	-2.869843	0.028869	-0.584777
N	1.652917	0.476610	-0.931348
O	-1.975267	-0.851648	-3.558390
O	-0.657821	0.787559	-2.809427
C	-2.064998	1.256802	-4.680326
C	-1.523856	0.329856	-3.620644
H	-1.375397	2.082531	-4.863391
H	-2.260209	0.705082	-5.602405
H	-3.017919	1.665708	-4.324222
Pd	-0.024712	-0.610467	-1.386207

TS3

SCF Done: -1349.578283 .a.u

C	-0.810530	-2.706989	-1.680781
H	-0.849947	-2.844742	-2.769104

H	-0.999069	-3.696300	-1.246113
C	-2.711373	-2.024814	-0.151494
C	-1.868401	-1.681056	-1.254626
H	-3.693186	-1.565041	-0.091636
H	-2.468181	-1.266529	-2.071761
N	0.791366	-0.996732	-1.100661
C	0.636963	-2.338658	-1.347378
O	1.536445	-3.174984	-1.344528
C	1.987452	-0.375210	-0.770555
C	1.884536	1.020850	-0.463600
C	3.249706	-0.963497	-0.699250
C	3.022640	1.783056	-0.072873
C	4.372654	-0.199599	-0.317508
H	3.344022	-2.015109	-0.925284
C	0.471705	2.874363	-0.237403
C	2.810591	3.150134	0.237458
C	4.282923	1.140969	-0.002008
H	5.337751	-0.696624	-0.267976
C	1.547896	3.695934	0.156863
H	-0.544220	3.247579	-0.318534
H	3.658850	3.758331	0.540735
H	5.157044	1.711379	0.297471
H	1.366927	4.739745	0.390140
N	0.642711	1.596202	-0.528797
Pd	-0.826959	0.136820	-0.900274
O	-2.445000	1.466324	-0.770398
O	-3.350622	0.872917	1.223251
C	-3.255601	1.606509	0.197114

C	-4.203249	2.790283	0.117519
H	-5.232267	2.445140	0.256494
H	-4.106447	3.310972	-0.836198
H	-3.981947	3.480762	0.939003
H	-2.667862	-3.028834	0.261641
H	-2.670137	-0.317848	1.401162
O	-2.252882	-1.306494	1.530453
C	-0.917550	-1.235900	1.880966
C	-0.369740	-0.018785	2.295822
C	-0.129147	-2.384320	1.808304
C	0.983277	0.041826	2.627991
H	-0.998922	0.862525	2.345700
C	1.225300	-2.304851	2.123352
H	-0.564246	-3.320536	1.475998
C	1.787264	-1.093759	2.532764
H	1.413071	0.991226	2.933900
H	1.846046	-3.189112	2.022141
H	2.847886	-1.031642	2.753280

TS4'

SCF Done: -1445.230484 .a.u

C	-1.047867	-1.131773	-1.177179
H	-1.036366	-1.149767	-2.274777
H	-1.984577	-1.617970	-0.877589
C	-0.940365	0.311552	-0.681981
H	-1.248510	1.074548	-1.395340
N	1.221902	-1.293686	-0.386246
C	0.112808	-2.029017	-0.722369
O	0.029445	-3.256699	-0.721017

C	2.474087	-1.803922	-0.078479
C	3.499284	-0.822159	0.153228
C	2.834396	-3.149109	0.007757
C	4.837762	-1.206101	0.456047
C	4.162827	-3.516976	0.309516
H	2.075284	-3.898033	-0.166352
C	4.044614	1.452299	0.266727
C	5.777423	-0.164139	0.664172
C	5.155407	-2.584543	0.532429
H	4.401832	-4.575774	0.366575
C	5.390018	1.154774	0.571173
H	3.671865	2.468871	0.179704
H	6.806957	-0.424693	0.896919
H	6.172510	-2.886143	0.765292
H	6.096722	1.963310	0.726520
N	3.150237	0.500007	0.070061
Pd	1.063768	0.695812	-0.323519
O	1.109888	2.770879	-0.286106
O	-1.083511	3.324850	-0.087381
C	0.119718	3.598683	-0.216874
C	0.562153	5.059903	-0.314076
H	-0.292775	5.727653	-0.189175
H	1.028098	5.239919	-1.289337
H	1.317503	5.275676	0.449251
C	-1.437913	0.556237	0.678747
H	-1.395598	-0.320873	1.327639
H	-1.081145	1.462093	1.153954
C	-3.992602	0.206581	-0.280712

C	-3.645772	0.746819	1.909154
C	-4.719884	-0.674658	0.542175
C	-4.104537	0.092346	-1.666380
H	-3.323575	1.167462	2.852729
N	-4.471266	-0.310539	1.881058
C	-5.522178	-1.696872	0.042040
C	-4.917315	-0.914412	-2.187055
H	-3.560417	0.764887	-2.320532
C	-4.972219	-1.045893	3.030975
C	-5.608027	-1.802507	-1.346125
H	-6.059749	-2.379129	0.692459
H	-5.012828	-1.021166	-3.263063
H	-4.562763	-2.061037	3.036667
H	-4.672172	-0.530042	3.944101
H	-6.063892	-1.099381	2.989291
H	-6.222744	-2.583510	-1.782284
C	-3.191424	1.080365	0.596848
H	-2.962044	2.108157	0.322602

TS4-HN-2A

SCF Done: -1216.198880 .a.u

C	1.222923	-3.323339	0.384802
H	1.397565	-4.343784	0.024573
H	1.147515	-3.381446	1.479414
C	-1.296320	-2.514091	0.503937
C	-0.061210	-2.741535	-0.201357
H	-2.220482	-2.787433	0.002860
H	-0.167426	-2.907787	-1.275447
N	2.153506	-1.152352	-0.112758

C	2.483335	-2.473293	0.073110
O	3.611511	-2.955190	0.068193
C	3.019498	-0.080958	-0.171912
C	2.394173	1.214195	-0.065363
C	4.406998	-0.128252	-0.305454
C	3.174727	2.407277	-0.124458
C	5.164743	1.060032	-0.352850
H	4.883959	-1.096683	-0.367858
C	0.419676	2.440223	0.197796
C	2.484552	3.641541	-0.026974
C	4.580134	2.307524	-0.273272
H	6.243053	0.980523	-0.462669
C	1.116348	3.664310	0.129058
H	-0.657737	2.404869	0.331678
H	3.053238	4.566693	-0.077041
H	5.175656	3.214451	-0.321675
H	0.570210	4.598843	0.203702
N	1.031675	1.271441	0.106358
Pd	0.185389	-0.719775	0.060219
H	-1.307395	-2.708328	1.573841
C	-1.877606	-0.597814	0.476870
C	-2.856390	-0.210292	-0.521850
C	-2.364192	-0.106958	1.677885
C	-3.876511	0.526000	0.141406
C	-2.960624	-0.415903	-1.904525
H	-1.953083	-0.202030	2.674275
N	-3.551719	0.571500	1.490808
C	-4.974012	1.064559	-0.535073

C	-4.056388	0.107099	-2.584193
H	-2.187115	-0.966398	-2.432963
C	-4.335283	1.233943	2.511613
C	-5.049388	0.842248	-1.907542
H	-5.740180	1.633325	-0.016299
H	-4.147129	-0.045708	-3.655649
H	-3.861975	1.075504	3.482663
H	-4.396616	2.312069	2.321666
H	-5.352188	0.826390	2.544899
H	-5.889170	1.244890	-2.466359

TS4-2A-OH

SCF Done: -1252.011764 .a.u

C	-1.144976	-3.341369	-0.224148
H	-1.222888	-4.338104	0.225285
H	-1.219117	-3.476566	-1.312026
C	1.294685	-2.455433	-0.751722
C	0.180700	-2.674664	0.134712
H	2.290072	-2.659509	-0.367213
H	0.442114	-2.758407	1.191662
N	-2.092182	-1.173043	0.252928
C	-2.386313	-2.514495	0.204044
O	-3.480924	-3.032692	0.399628
C	-2.987916	-0.130556	0.362826
C	-2.441247	1.174242	0.082865
C	-4.339954	-0.215748	0.694535
C	-3.258027	2.340901	0.172361
C	-5.135476	0.946089	0.769736
H	-4.760394	-1.192953	0.888254

C	-0.578787	2.445273	-0.538776
C	-2.643449	3.587921	-0.104028
C	-4.623302	2.203938	0.525169
H	-6.183452	0.837667	1.036444
C	-1.312641	3.646401	-0.453773
H	0.469836	2.437704	-0.822167
H	-3.240055	4.494127	-0.035610
H	-5.245751	3.091016	0.597017
H	-0.824115	4.591311	-0.667519
N	-1.119684	1.265719	-0.283595
Pd	-0.187792	-0.686781	-0.223810
H	1.166831	-2.727948	-1.796735
C	1.791002	-0.527702	-0.936786
C	2.885689	-0.046077	-0.114184
C	2.074399	-0.097959	-2.224400
C	3.769656	0.682036	-0.957065
C	3.183918	-0.177245	1.247680
H	1.524579	-0.271667	-3.139323
N	3.242037	0.631794	-2.242457
C	4.927170	1.284673	-0.467433
C	4.345258	0.414418	1.737190
H	2.525527	-0.712066	1.924229
C	5.206613	1.141598	0.888585
H	5.596599	1.846540	-1.112741
H	6.103296	1.597977	1.302545
O	4.613763	0.266216	3.074176
H	5.436624	0.734015	3.282195
H	3.662771	1.041851	-3.061936

TS4-N-2A

SCF Done: -1232.161180 .a.u

C	1.239088	-3.326096	0.378926
H	1.420434	-4.345265	0.018660
H	1.161370	-3.384960	1.473275
C	-1.285038	-2.529689	0.492447
C	-0.046736	-2.751530	-0.210574
H	-2.206052	-2.817219	-0.006841
H	-0.150236	-2.921045	-1.284465
N	2.157417	-1.148727	-0.114824
C	2.494941	-2.468115	0.070288
O	3.625915	-2.942523	0.066855
C	3.017053	-0.071391	-0.169979
C	2.383677	1.219215	-0.060036
C	4.404756	-0.110231	-0.301732
C	3.157258	2.417101	-0.112289
C	5.155646	1.082731	-0.343489
H	4.887721	-1.075514	-0.366550
C	0.401992	2.432815	0.207001
C	2.460060	3.646895	-0.009261
C	4.563449	2.326232	-0.259528
H	6.234525	1.009999	-0.451902
C	1.091630	3.661143	0.145963
H	-0.675227	2.391802	0.340761
H	3.023478	4.575502	-0.053757
H	5.153621	3.236861	-0.302861
H	0.539974	4.591920	0.225885
N	1.020325	1.267696	0.109188

Pd	0.187840	-0.728629	0.052298
H	-1.295558	-2.720094	1.563120
C	-1.880332	-0.623810	0.457672
C	-2.845214	-0.229152	-0.546398
C	-2.378884	-0.127899	1.654857
C	-3.866661	0.514870	0.109547
C	-2.984358	-0.396712	-1.927204
H	-1.974772	-0.229013	2.653531
N	-3.558068	0.560929	1.460634
C	-4.100680	0.171549	-2.538908
H	-2.241490	-0.943090	-2.502033
C	-4.357356	1.231699	2.469075
C	-5.033632	0.891244	-1.770793
H	-4.256888	0.071774	-3.608187
H	-4.679127	0.525391	3.241561
H	-3.790699	2.042804	2.939031
H	-5.234150	1.646701	1.969957
H	-5.900981	1.339922	-2.249934
N	-4.935084	1.076596	-0.448331

TS4-HO-2A

SCF Done: -1252.619627 .a.u

C	0.950597	-3.321250	0.042473
H	1.058938	-4.319109	-0.398522
H	0.882136	-3.458496	1.130325
C	-1.517919	-2.388284	0.253496
C	-0.300165	-2.618065	-0.478427
H	-2.455543	-2.551256	-0.271863
H	-0.418929	-2.681686	-1.562011

N	2.004820	-1.177144	-0.293789
C	2.256106	-2.526238	-0.221530
O	3.352936	-3.072287	-0.285829
C	2.934622	-0.159339	-0.274369
C	2.392186	1.156209	-0.041506
C	4.314739	-0.278125	-0.437571
C	3.243853	2.300714	-0.009547
C	5.143586	0.861773	-0.393860
H	4.730114	-1.264147	-0.593832
C	0.501024	2.469918	0.367141
C	2.632489	3.560490	0.210123
C	4.638243	2.130192	-0.193360
H	6.213411	0.727561	-0.530422
C	1.270573	3.651187	0.393644
H	-0.574540	2.487951	0.517637
H	3.256290	4.450573	0.231484
H	5.287895	3.000274	-0.172466
H	0.783921	4.606285	0.561436
N	1.038294	1.279316	0.161028
Pd	0.071340	-0.642914	-0.038170
H	-1.535511	-2.675975	1.302467
C	-1.963646	-0.449651	0.446661
C	-2.980211	0.091472	-0.445578
C	-2.418408	-0.152894	1.716972
C	-3.996183	0.690038	0.344887
C	-3.115289	0.107351	-1.838420
N	-3.645358	0.492112	1.687325
C	-5.107494	1.318587	-0.207144

C	-4.231278	0.723517	-2.403392
H	-2.347457	-0.340094	-2.463288
C	-5.211375	1.328672	-1.599445
H	-5.868363	1.780299	0.416364
H	-4.342078	0.745058	-3.483641
H	-6.065410	1.811191	-2.065327
O	-1.826241	-0.470121	2.891788
H	-2.503386	-0.604246	3.575529
H	-3.997278	1.061484	2.444819

TS5-HN-2A

SCF Done: -1216.117071 .a.u

C	-1.164405	2.774870	1.778550
H	-1.345102	3.855978	1.767295
H	-1.072058	2.479215	2.832730
C	1.356772	1.983861	1.595153
C	0.110763	2.418802	1.018129
H	2.272920	2.408496	1.194870
H	0.200229	2.921361	0.052717
N	-2.101548	0.873166	0.624418
C	-2.429089	2.062883	1.228992
O	-3.557438	2.514760	1.395324
C	-2.967837	-0.127331	0.237282
C	-2.340313	-1.384811	-0.086384
C	-4.357264	-0.047238	0.146152
C	-3.121115	-2.500119	-0.513743
C	-5.115081	-1.161630	-0.268921
H	-4.835601	0.887436	0.404656
C	-0.361383	-2.619727	-0.259169

C	-2.428918	-3.696670	-0.827404
C	-4.528709	-2.365539	-0.602248
H	-6.195003	-1.056954	-0.331744
C	-1.058448	-3.760853	-0.706826
H	0.717960	-2.623334	-0.136697
H	-2.997867	-4.559954	-1.163341
H	-5.124473	-3.212240	-0.930373
H	-0.510769	-4.666971	-0.943871
N	-0.975288	-1.486713	0.038074
Pd	-0.130777	0.418657	0.620858
H	1.384345	1.824717	2.670540
C	1.938490	0.180703	0.946331
C	2.901854	0.139320	-0.138035
C	2.443879	-0.666797	1.919197
C	3.932492	-0.765259	0.239064
C	2.984533	0.778127	-1.383033
H	2.048226	-0.898578	2.899289
N	3.628688	-1.242943	1.507121
C	5.019628	-1.052411	-0.590306
C	4.069876	0.506723	-2.210407
H	2.202657	1.464824	-1.695642
C	4.428307	-2.193545	2.249960
C	5.073604	-0.401217	-1.819862
H	5.794023	-1.753354	-0.292604
H	4.143916	0.995620	-3.177413
H	3.970040	-2.357517	3.227285
H	4.487205	-3.153430	1.723321
H	5.445410	-1.812687	2.397446

H	5.904812	-0.598775	-2.490454
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TS5-2A-OH

SCF Done: -1252.013560 .a.u

C	-1.152385	2.774366	1.776451
H	-1.333839	3.855317	1.763746
H	-1.061447	2.479721	2.831044
C	1.369004	1.983405	1.597176
C	0.123971	2.418602	1.018136
H	2.284913	2.408748	1.196573
H	0.215082	2.920379	0.052522
N	-2.085920	0.871320	0.621736
C	-2.415523	2.060905	1.225596
O	-3.544632	2.511344	1.390438
C	-2.950931	-0.129471	0.232675
C	-2.322243	-1.386672	-0.089697
C	-4.340208	-0.049867	0.138509
C	-3.101806	-2.502259	-0.518624
C	-5.096733	-1.164475	-0.278259
H	-4.819457	0.884628	0.395927
C	-0.342668	-2.621056	-0.257894
C	-2.408646	-3.698647	-0.830618
C	-4.509233	-2.368208	-0.610210
H	-6.176542	-1.060104	-0.343537
C	-1.038461	-3.762446	-0.706867
H	0.736321	-2.624885	-0.132422
H	-2.976655	-4.562114	-1.167691
H	-5.103956	-3.215143	-0.939631
H	-0.490012	-4.668522	-0.942299

N	-0.957440	-1.488040	0.037682
Pd	-0.114821	0.418332	0.620769
H	1.395469	1.826499	2.672974
C	1.954986	0.183935	0.952769
C	2.924858	0.153069	-0.126755
C	2.449622	-0.673669	1.923744
C	3.953797	-0.755391	0.244697
C	3.003334	0.817468	-1.356891
H	2.042751	-0.911125	2.897208
N	3.630654	-1.244898	1.505292
C	5.041600	-1.018092	-0.586220
C	4.094550	0.565179	-2.183931
H	2.229658	1.505687	-1.680946
C	5.102021	-0.346675	-1.803961
H	5.822268	-1.718358	-0.302605
H	5.938957	-0.527411	-2.475198
O	4.146947	1.233095	-3.380898
H	4.943363	0.956992	-3.859119
H	4.187530	-1.894299	2.039030

TS5-N-2A

SCF Done: -1232.158821 .a.u

C	-1.197145	2.766566	1.810693
H	-1.386384	3.846180	1.812411
H	-1.102720	2.458777	2.861148
C	1.330274	1.996204	1.618170
C	0.080780	2.430116	1.046043
H	2.242818	2.440113	1.230312
H	0.167335	2.947806	0.088340

N	-2.117908	0.870599	0.633596
C	-2.455605	2.050864	1.251584
O	-3.587597	2.491138	1.421673
C	-2.975786	-0.133357	0.235116
C	-2.337796	-1.382420	-0.099138
C	-4.365440	-0.063067	0.142875
C	-3.109305	-2.500399	-0.536156
C	-5.114111	-1.179726	-0.282920
H	-4.851587	0.865288	0.409419
C	-0.349421	-2.601236	-0.278186
C	-2.407749	-3.689346	-0.857583
C	-4.517805	-2.376028	-0.625442
H	-6.194698	-1.082976	-0.346127
C	-1.037061	-3.744389	-0.734766
H	0.729632	-2.599156	-0.153226
H	-2.969626	-4.554417	-1.200623
H	-5.106457	-3.224727	-0.961037
H	-0.482080	-4.644722	-0.976537
N	-0.971891	-1.474439	0.025567
Pd	-0.145021	0.433248	0.624393
H	1.356838	1.819849	2.690970
C	1.929387	0.214732	0.943353
C	2.879605	0.183447	-0.147983
C	2.447467	-0.647366	1.900490
C	3.912759	-0.728853	0.209073
C	2.997079	0.801603	-1.396240
H	2.058549	-0.887021	2.881402
N	3.625117	-1.223782	1.472043

C	4.105166	0.477243	-2.177402
H	2.244181	1.502576	-1.746367
C	4.441396	-2.185830	2.188911
C	5.051505	-0.450060	-1.705264
H	4.244656	0.928014	-3.154674
H	4.773384	-1.774226	3.147821
H	3.883928	-3.111166	2.370111
H	5.311361	-2.404840	1.568179
H	5.912413	-0.707540	-2.318229
N	4.973766	-1.065298	-0.518500

TS5-HO-2A

SCF Done: -1252.013893 .a.u

C	-1.150720	2.739644	1.810952
H	-1.333657	3.820437	1.829864
H	-1.032988	2.417286	2.854585
C	1.370647	1.976053	1.549861
C	0.106151	2.404297	1.012185
H	2.269908	2.406681	1.116748
H	0.164901	2.920019	0.051516
N	-2.107968	0.861461	0.637174
C	-2.425040	2.037952	1.272591
O	-3.550665	2.484300	1.470278
C	-2.981256	-0.134063	0.253593
C	-2.359695	-1.386693	-0.098131
C	-4.372305	-0.053798	0.190280
C	-3.147811	-2.496966	-0.525231
C	-5.137292	-1.163196	-0.224806
H	-4.846011	0.876871	0.470725

C	-0.384014	-2.617552	-0.323940
C	-2.461097	-3.688769	-0.867412
C	-4.556859	-2.362198	-0.585295
H	-6.218307	-1.058583	-0.265420
C	-1.088606	-3.753244	-0.773450
H	0.697402	-2.622161	-0.222303
H	-3.035762	-4.548120	-1.203727
H	-5.158370	-3.204995	-0.913021
H	-0.544825	-4.655729	-1.032331
N	-0.992528	-1.489015	-0.000228
Pd	-0.138623	0.404148	0.596785
H	1.427794	1.802801	2.622304
C	1.926130	0.167999	0.904367
C	2.921682	0.117654	-0.158012
C	2.461202	-0.597147	1.922608
C	4.007186	-0.683358	0.284003
C	2.984750	0.690761	-1.433189
N	3.716858	-1.085286	1.594939
C	5.119480	-0.947699	-0.508305
C	4.100391	0.443347	-2.232200
H	2.163196	1.303065	-1.794251
C	5.151162	-0.371713	-1.779773
H	5.934761	-1.572863	-0.154259
H	4.155806	0.879881	-3.225198
H	6.003757	-0.557100	-2.426270
O	1.915255	-0.837923	3.137291
H	2.619157	-0.953355	3.796997
H	4.136874	-1.891953	2.036191

2a-HN-2A

SCF Done: -1090.614803 .a.u

C	-0.787878	-3.418182	0.632941
H	-0.142820	-2.536960	0.739926
H	-0.867748	-3.875984	1.628645
C	1.182974	-4.969318	0.158579
H	1.883369	-4.134650	0.295828
C	-2.197532	-3.027114	0.207134
O	-3.034280	-3.866133	-0.103654
C	-3.616415	-0.999487	-0.102691
C	-3.547888	0.429687	0.010031
C	-4.799995	-1.598322	-0.499852
C	-4.701503	1.214517	-0.288524
C	-5.930948	-0.801344	-0.790415
H	-4.842522	-2.674704	-0.583013
C	-2.288918	2.290201	0.510368
C	-4.570738	2.619401	-0.158590
C	-5.898436	0.571058	-0.691975
H	-6.845750	-1.298831	-1.099520
C	-3.370243	3.160753	0.239302
H	-1.329567	2.696350	0.826696
H	-5.426569	3.253337	-0.376646
H	-6.774724	1.171932	-0.918419
H	-3.241276	4.232953	0.347337
N	-2.365071	0.977791	0.402938
C	1.784265	-5.981916	-0.768241
C	1.290926	-7.313282	-1.023591
C	2.886776	-5.823301	-1.569495

C	2.152044	-7.901240	-1.992625
C	0.215592	-8.066614	-0.526540
H	1.038590	-5.414220	1.154339
H	3.543662	-4.969834	-1.675468
C	1.964312	-9.203212	-2.466636
C	0.024585	-9.361038	-0.994792
H	-0.458690	-7.643415	0.212960
C	0.889442	-9.922811	-1.955220
H	2.630182	-9.639040	-3.205856
H	-0.805543	-9.951467	-0.617762
H	0.713744	-10.936843	-2.302990
C	4.198164	-7.177335	-3.254107
H	3.808314	-7.402882	-4.253918
H	4.799295	-6.267549	-3.312594
H	4.845344	-8.004385	-2.937593
N	3.120749	-6.970387	-2.313581
C	-0.167966	-4.428196	-0.339045
H	-0.029894	-3.961518	-1.322464
H	-0.875412	-5.250225	-0.483350
N	-2.436128	-1.674143	0.210715
H	-1.689422	-1.040321	0.478909

2a-2A-OH

SCF Done: -1126.511991 .a.u

C	-0.773301	-3.405096	0.517333
H	-0.123610	-2.525792	0.613128
H	-0.860920	-3.843293	1.521559
C	1.203573	-4.954897	0.071745
H	1.900247	-4.112883	0.180279

C	-2.177258	-3.007813	0.077342
O	-3.000165	-3.836635	-0.291124
C	-3.610833	-0.979854	-0.154283
C	-3.559063	0.442443	0.031483
C	-4.781845	-1.569018	-0.600399
C	-4.715943	1.230306	-0.245939
C	-5.916251	-0.769217	-0.868717
H	-4.811955	-2.640173	-0.738434
C	-2.327651	2.287356	0.645513
C	-4.601837	2.628011	-0.043280
C	-5.899621	0.596720	-0.700777
H	-6.820864	-1.259255	-1.217230
C	-3.413514	3.160097	0.400957
H	-1.377727	2.686165	0.997642
H	-5.460684	3.263897	-0.243076
H	-6.778407	1.199883	-0.910890
H	-3.297466	4.226660	0.565003
N	-2.388429	0.981402	0.470821
C	1.803686	-5.990669	-0.829724
C	1.328998	-7.340381	-1.015908
C	2.881783	-5.840375	-1.666891
C	2.171873	-7.954729	-1.983561
C	0.279055	-8.077129	-0.446949
H	1.069601	-5.373098	1.080335
H	3.514869	-4.977075	-1.821255
C	1.984871	-9.276617	-2.386892
C	0.095065	-9.394734	-0.848761
H	-0.389555	-7.647660	0.291748

C	0.939115	-9.989657	-1.810476
H	2.630102	-9.743088	-3.126142
H	0.767391	-11.023330	-2.104121
N	3.109628	-7.011699	-2.366204
C	-0.153535	-4.435223	-0.432098
H	-0.022899	-3.991880	-1.427218
H	-0.856445	-5.264690	-0.553907
N	-2.428866	-1.658320	0.143447
H	-1.693167	-1.032230	0.456525
O	-0.938328	-10.095187	-0.272697
H	-0.959670	-10.984805	-0.655811
H	3.854479	-7.161633	-3.026930

2a-N-2A .a.u

SCF Done: -1106.657769

C	-0.759198	-3.374959	0.599839
H	-0.112178	-2.491850	0.673145
H	-0.826651	-3.802875	1.609909
C	1.190507	-4.961648	0.155623
H	1.903072	-4.134723	0.274761
C	-2.174511	-2.993936	0.181336
O	-3.004639	-3.839381	-0.130500
C	-3.615141	-0.978107	-0.101283
C	-3.558843	0.450386	0.024260
C	-4.795693	-1.584539	-0.495340
C	-4.721765	1.227065	-0.258653
C	-5.936217	-0.795584	-0.770330
H	-4.828921	-2.660443	-0.588310
C	-2.313356	2.317680	0.532606

C	-4.603019	2.631875	-0.116762
C	-5.915570	0.576054	-0.659372
H	-6.848577	-1.298690	-1.077461
C	-3.404634	3.180579	0.277386
H	-1.355512	2.729826	0.845642
H	-5.466147	3.259869	-0.322808
H	-6.799015	1.170733	-0.873973
H	-3.284680	4.252874	0.394291
N	-2.378190	1.005635	0.413649
C	1.777407	-5.998752	-0.753371
C	1.249541	-7.311116	-1.020934
C	2.908812	-5.882905	-1.525452
C	2.121000	-7.929760	-1.964785
C	0.154578	-8.069020	-0.590753
H	1.042841	-5.385043	1.160308
H	3.594145	-5.049874	-1.611450
C	0.008715	-9.350652	-1.115176
H	-0.560349	-7.674069	0.125891
C	0.944272	-9.841093	-2.044259
H	0.827316	-10.842317	-2.453872
N	3.129410	-7.036965	-2.260160
C	-0.154379	-4.413733	-0.350163
H	-0.014283	-3.971708	-1.344507
H	-0.874229	-5.228494	-0.473341
N	-2.425635	-1.644206	0.197078
H	-1.683393	-1.004974	0.465350
C	4.221152	-7.289293	-3.177882
H	5.186597	-7.237692	-2.662199

H	4.083268	-8.293119	-3.582342
H	4.216286	-6.565170	-4.000150
N	2.004152	-9.151732	-2.481029
H	-0.824039	-9.979220	-0.816265

2a-HO-2A

SCF Done: -1126.510367 .a.u

C	-0.788429	-3.431651	0.641364
H	-0.140354	-2.553018	0.749868
H	-0.863249	-3.897014	1.633874
C	1.175926	-4.981821	0.144670
H	1.880710	-4.152062	0.278766
C	-2.199937	-3.035829	0.227103
O	-3.045334	-3.872897	-0.065454
C	-3.608254	-1.002786	-0.094063
C	-3.529871	0.427188	0.001047
C	-4.798921	-1.598662	-0.474265
C	-4.680924	1.215780	-0.297556
C	-5.927183	-0.797996	-0.765041
H	-4.848727	-2.675659	-0.544290
C	-2.254992	2.285431	0.468368
C	-4.540127	2.621264	-0.185835
C	-5.885216	0.575256	-0.683387
H	-6.847625	-1.293270	-1.060708
C	-3.332950	3.159624	0.195527
H	-1.290429	2.689104	0.771737
H	-5.393665	3.258033	-0.404664
H	-6.759515	1.179003	-0.909915
H	-3.196220	4.232215	0.289265

N	-2.340474	0.972372	0.377675
C	1.771256	-5.981805	-0.796034
C	1.309778	-7.328815	-1.052541
C	2.864935	-5.804090	-1.597853
C	2.184259	-7.910241	-2.011052
C	0.251514	-8.097723	-0.548081
H	1.035991	-5.439689	1.135117
C	2.013695	-9.209304	-2.484925
C	0.076189	-9.396102	-1.017433
H	-0.427027	-7.682375	0.191739
C	0.943189	-9.944452	-1.979187
H	2.690092	-9.634954	-3.221284
H	0.779426	-10.958385	-2.332474
N	3.163906	-6.966389	-2.305642
C	-0.176509	-4.435244	-0.342479
H	-0.041283	-3.959986	-1.321919
H	-0.886781	-5.254761	-0.489215
N	-2.429822	-1.681368	0.217430
H	-1.675903	-1.049522	0.469587
H	3.695737	-6.954668	-3.164126
H	-0.745728	-9.996562	-0.638195
O	3.619031	-4.681426	-1.771119
H	4.543282	-4.883325	-1.548052