Design and Validation of Non-Metal Oxo Complexes for C-H Activation

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S.1 Computational details

The geometry optimizations were carried out using the B3LYP functional[1-3] with the 6-31G** basis set[4-5] for all atoms except the metals. For metals we used the small core angular momentum projected effective core potential (ECP)[6] from Los Alamos,[7] for which the outer core and valence electrons described explicitly using the double-ζ contraction of valence functions plus polarization. Thus a neural V, Nb, or Ta is described with 13 explicit electrons while Ni, Pd, Pt are described with 18 explicit electrons.

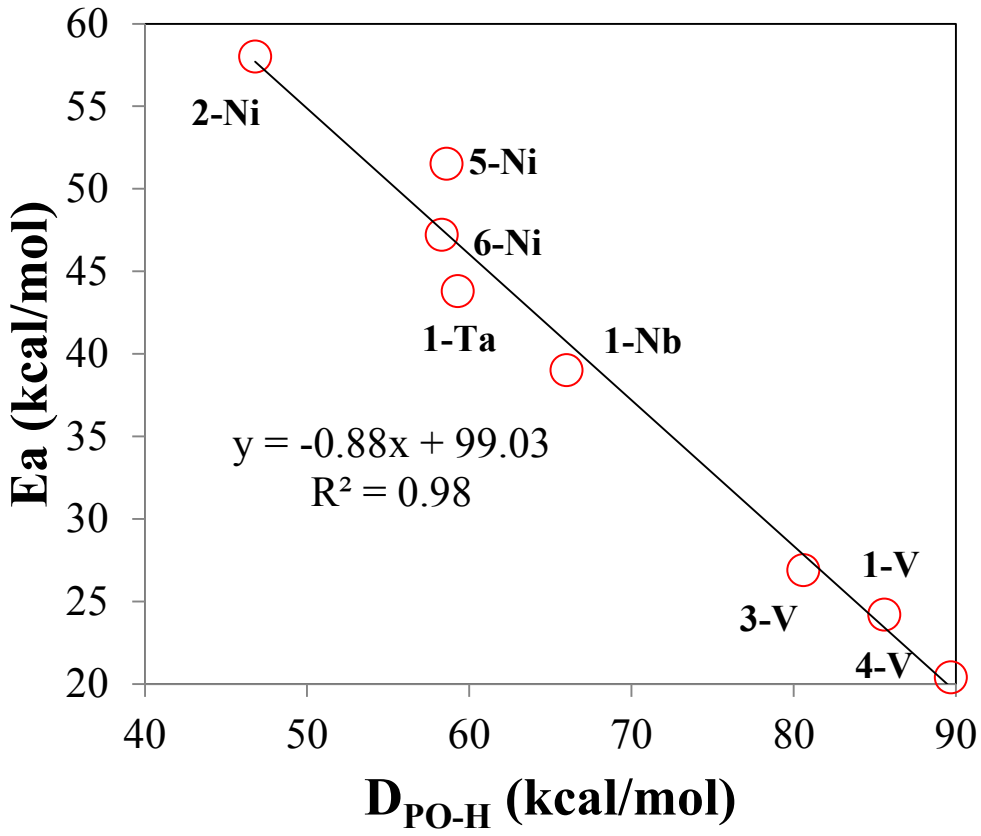
To obtain the most accurate energetics, we finished by calculating at the single optimum geometry-point the energy using the same functional but with a larger basis set: metals were described with the triple-ζ contraction of valence functions augmented with two *f*-functions[8] but with the core electrons described by the same small core ECP; while the other atoms are described with the 6-311++G** basis set.

The analytic Hessian was calculated for each local minimum and each transition state and used to calculate the vibrational frequencies. The calculated zero-point vibrational energy is not included in the potential energy surface. The discussion of energies in the manuscript is all based on the electronic energy. We ensured that each local minimum had zero imaginary frequencies, while each transition state structure had exactly one imaginary frequency. All calculations were performed using the Jaguar 7.6 program package.

S.2 Correlation between D_{PO-H} and E_a

By analyzing D_{PO-H}'s and E_a's, we found that there is an excellent correlation ($R^2 = 0.98$) between two. The reason for this good correlation is because during the ROA pathway a C-H bond is broken and a PO-H bond is formed, and therefore if the same alkane is activated the C-H cleavage barrier depends on the strength of the PO-H bond. This validates our assertion that E_a can be estimated by simply calculating D_{PO-H}, at least in this type of C-H activation pathway.

(a)



(b)

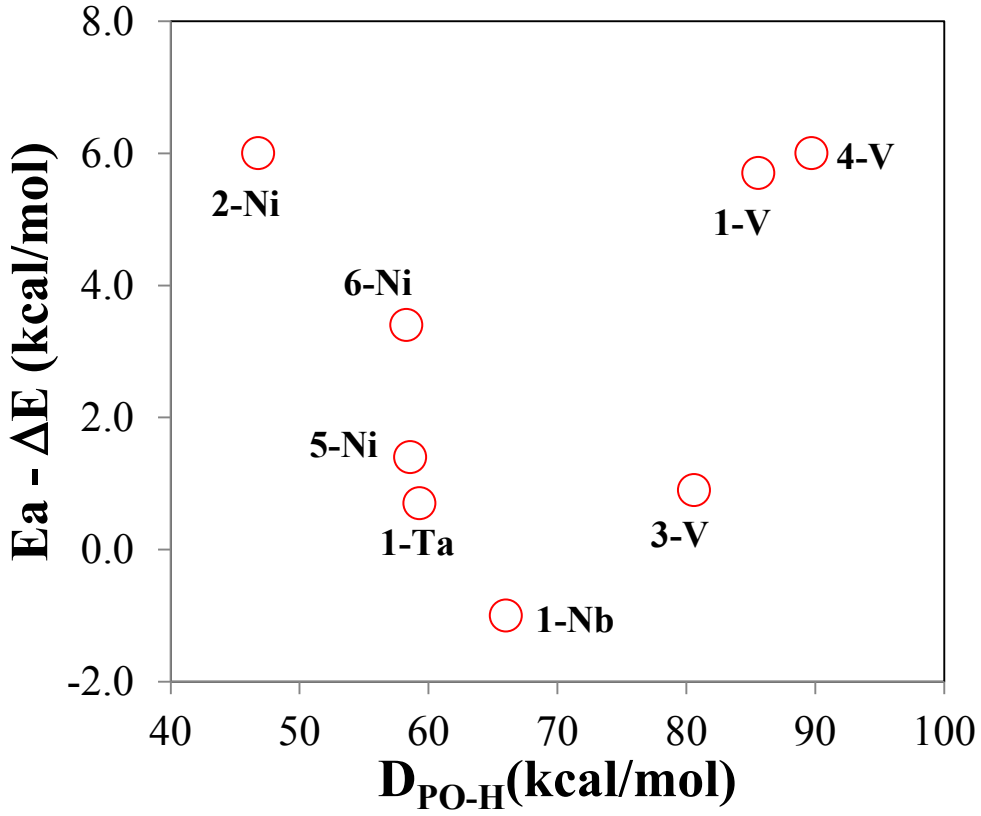


Figure S1. Illustrates that a rapid assay for good catalysts can focus on D_{PO-H}.

(a) Comparson of E_a with $D_{PO-H.}$

(b) Comparison of (Ea-ΔE) with D_{PO-H} , where $\Delta E = D_{C-H} - D_{PO-H}$ is the reaction energy

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S.3 Coordinates for optimized structures

1^3-V

E(SCF)= -2021.30782461174

C1	-3.5039554327	-1.4832474332	-0.1544291967
C2	-4.7431186129	-1.7802797580	-0.7282894245
C3	-2.7526224774	-2.4733278094	0.5027914472
C4	-5.2241307562	-3.0835437864	-0.6203359763
H5	-5.2969104584	-1.0039630749	-1.2445377679
C6	-3.2582175810	-3.7712854273	0.6185086109
C7	-4.4939587569	-4.0746998551	0.0479685560
H8	-6.1840006871	-3.3331677707	-1.0629821204
H9	-2.6984136473	-4.5361560668	1.1485617893
H10	-4.8915240944	-5.0819368746	0.1249324863
C11	0.9998586206	-1.4718657323	-0.1393630022
C12	2.2450701876	-1.7622757642	-0.7035052162
C13	0.2507826659	-2.4649385884	0.5159159993
C14	2.7339722995	-3.0619564076	-0.5884878626
H15	2.7973010227	-0.9836819423	-1.2179983190
C16	0.7646007965	-3.7590051079	0.6396359363
C17	2.0059410812	-4.0559493216	0.0779590600
H18	3.6984524706	-3.3064691298	-1.0238931794
H19	0.2066677311	-4.5257352968	1.1689550297
H20	2.4096300097	-5.0602993862	0.1605609195
P21	-1.2559954289	-1.7651978515	1.2253768230
Cl22	-1.2628365634	2.1368066612	0.8287226840
Cl23	-1.2524203090	0.2809843157	-2.4475218290
O24	-1.2632239524	-1.5812931761	2.7164632333
O25	-2.9799583724	-0.2360633129	-0.2129830680
O26	0.4679484089	-0.2286113232	-0.2060370947
V27	-1.2570338837	0.2821373675	-0.2433207849

1^3-Nb

E(SCF)= -2006.34766671290

C1	-3.5734735055	-1.5454253979	-0.1350745873
C2	-4.8335892807	-1.8598932621	-0.6450275695
C3	-2.7687744230	-2.5225248387	0.4814517082
C4	-5.2891300333	-3.1720372468	-0.5306562474
H5	-5.4267112687	-1.0860378060	-1.1202632025
C6	-3.2532417565	-3.8298950851	0.6008284226
C7	-4.5073839091	-4.1553742739	0.0864137257
H8	-6.2665101498	-3.4314669846	-0.9268858655
H9	-2.6558025223	-4.5891121134	1.0969283307
H10	-4.8792875573	-5.1719088238	0.1687947887
C11	1.0697497507	-1.5323791645	-0.1177767626
C12	2.3355193048	-1.8398957117	-0.6179229625
C13	0.2662121775	-2.5138624465	0.4932290889
C14	2.7979721460	-3.1492320643	-0.4989299342
H15	2.9276192433	-1.0629537937	-1.0893660771
C16	0.7576148956	-3.8182139894	0.6176540568
C17	2.0175041095	-4.1366277937	0.1130874832
H18	3.7798649621	-3.4030176929	-0.8875128839
H19	0.1611385041	-4.5805373511	1.1100969519
H20	2.3949058238	-5.1508194698	0.1992544767
P21	-1.2559891877	-1.8121699935	1.1946424124
Cl22	-1.2664292147	2.3018979965	0.9537498347
Cl23	-1.2486052852	0.3594549852	-2.6055245103
O24	-1.2621928806	-1.6782419529	2.6977564610
O25	-3.0919907242	-0.2698640718	-0.2358371762
O26	0.5815621887	-0.2597329054	-0.2230241248
Nb27	-1.2568273671	0.3485726072	-0.2649197812

1^3-Ta

E(SCF)= -2007.87751751980

C1	-3.5790803107	-1.5429550194	-0.1355656543
C2	-4.8495685801	-1.8407666796	-0.6230842893
C3	-2.7761921693	-2.5256847294	0.4746529767
C4	-5.3210117355	-3.1471809101	-0.4959417492
H5	-5.4418544769	-1.0619133790	-1.0911097445
C6	-3.2771805456	-3.8252310264	0.6063899290
C7	-4.5428544170	-4.1376384932	0.1121350227
H8	-6.3085015963	-3.3944873962	-0.8744284432
H9	-2.6822239379	-4.5893839834	1.0983163150
H10	-4.9265964276	-5.1490380063	0.2046783903

C11	1.0751077656	-1.5301096947	-0.1180892044
C12	2.3509827242	-1.8206128809	-0.5956782336
C13	0.2734602255	-2.5172520338	0.4866089425
C14	2.8293014337	-3.1240609048	-0.4640414432
H15	2.9422134533	-1.0385353455	-1.0596555854
C16	0.7813806884	-3.8136683253	0.6233373775
C17	2.0526163340	-4.1187942970	0.1389264663
H18	3.8210962411	-3.3657112487	-0.8348421568
H19	0.1872932066	-4.5809049567	1.1114771611
H20	2.4417376943	-5.1277881692	0.2352373816
P21	-1.2560997185	-1.8195727576	1.1854678514
Cl22	-1.2664014242	2.2469670845	0.9733875191
Cl23	-1.2486308746	0.3607811692	-2.6012636111
O24	-1.2621726584	-1.7228816124	2.6940903798
O25	-3.0773971991	-0.2674256375	-0.2517312189
O26	0.5668651050	-0.2575925046	-0.2387324831
Ta27	-1.2567567215	0.3217649518	-0.2664383783

2^1-Ni

E(SCF)= -2351.02183384777

P1	0.9563717564	0.3125662239	0.1383607424
P2	-3.3920588377	0.1520444306	-0.3767521544
C3	-3.7891930858	-1.6231296656	-0.1039739820
C4	-5.0286948903	-2.2106004002	-0.3930861164
C5	-2.7715746056	-2.3886339724	0.4913944553
C6	-5.2563277553	-3.5490481308	-0.0790900874
H7	-5.8211760798	-1.6252947487	-0.8530738650
C8	-3.0266506138	-3.7209728101	0.8462417367
C9	-4.2586582565	-4.3004325141	0.5493242852
H10	-6.2169526686	-4.0032733772	-0.3058906512
H11	-2.2699922709	-4.2942338413	1.3742764991
H12	-4.4484599722	-5.3365709044	0.8161549120
C13	1.2434725233	-1.4430695613	-0.3439425339
C14	2.3905837769	-1.9248958129	-0.9818199573
C15	0.1674718937	-2.3140804156	-0.0667185276
C16	2.4684047368	-3.2682141069	-1.3544956715
H17	3.2202552884	-1.2585364515	-1.2023067943
C18	0.2616002730	-3.6587802678	-0.4376924134
C19	1.4044841741	-4.1304368366	-1.0870309532
H20	3.3558490429	-3.6390147330	-1.8600389515
H21	-0.5608401355	-4.3391114805	-0.2405703235
H22	1.4629102977	-5.1728821108	-1.3884007894
C23	-4.5882057786	1.0985367222	0.6533340755

H24	-4.3771873174	2.1621005837	0.5131854591
H25	-5.6239658344	0.8849138047	0.3721710126
H26	-4.4373997462	0.8473286822	1.7058210053
C27	-3.8921606802	0.5379451633	-2.1042948389
H28	-4.9630895888	0.3775386856	-2.2619599030
H29	-3.6376951375	1.5833696411	-2.2942522961
H30	-3.3247266158	-0.0895009020	-2.7957509141
C31	1.7478229425	0.5285508260	1.7865799249
H32	2.8100046319	0.2671898013	1.7626821939
H33	1.6350037336	1.5722131041	2.0947288754
H34	1.2168998522	-0.1129949154	2.4951028513
C35	1.9497399804	1.3489067681	-1.0077127966
H36	1.7046843035	2.3943847948	-0.8059067842
H37	3.0240128455	1.1866197409	-0.8773469430
H38	1.6631284514	1.1306214967	-2.0389300413
P39	-1.1931214729	-1.5251989675	0.9249890842
Cl40	-1.3551507848	2.6529591039	-0.6601240788
Ni41	-1.2631971530	0.4996526663	0.0468780955
O42	-0.8980072585	-1.6511871227	2.4104834393

2^1-Pd

E(SCF)= -2308.45974535869

P1	1.0655308615	0.2996990041	0.1697087749
P2	-3.5113717295	0.1540456806	-0.3621959107
C3	-3.8149171872	-1.6444633128	-0.1032875583
C4	-5.0383108273	-2.2586798565	-0.4070289993
C5	-2.7846365823	-2.3968059120	0.4903226554
C6	-5.2431331623	-3.6043572739	-0.1097386961
H7	-5.8398968876	-1.6852161662	-0.8659760880
C8	-3.0206129820	-3.7366776818	0.8327721126
C9	-4.2371669465	-4.3402397887	0.5214733265
H10	-6.1927970550	-4.0740032891	-0.3502337283
H11	-2.2583852064	-4.2981522510	1.3652577141
H12	-4.4069093535	-5.3818141087	0.7799380332
C13	1.2753942874	-1.4720896484	-0.2998873442
C14	2.4218256583	-1.9802944241	-0.9191533837
C15	0.1804997203	-2.3250140579	-0.0355253480
C16	2.4833003004	-3.3248396537	-1.2893640441
H17	3.2674185065	-1.3303930281	-1.1277397764
C18	0.2591631474	-3.6718511524	-0.4039281561
C19	1.4010491054	-4.1668986690	-1.0368668963
H20	3.3720808768	-3.7109997396	-1.7805270531
H21	-0.5764842888	-4.3381259195	-0.2156891102
H22	1.4433813785	-5.2109164389	-1.3351607801

C23	-4.7488026385	1.0173697685	0.6929853284
H24	-4.6133282041	2.0940057858	0.5570893254
H25	-5.7731451007	0.7391633487	0.4260681262
H26	-4.5657998843	0.7709247144	1.7414240391
C27	-4.0425100464	0.5461010302	-2.0779117728
H28	-5.1145180068	0.3804873162	-2.2230720963
H29	-3.7947891518	1.5950710210	-2.2616158618
H30	-3.4774742405	-0.0694751706	-2.7815632254
C31	1.8995428810	0.4783683851	1.8018588630
H32	2.9473818034	0.1666254384	1.7539461724
H33	1.8431374942	1.5243222431	2.1167877217
H34	1.3593229760	-0.1411047823	2.5228263420
C35	2.0744333828	1.2896668460	-1.0025532445
H36	1.8494334427	2.3440612854	-0.8234110841
H37	3.1468071409	1.1109038204	-0.8779986726
H38	1.7728283205	1.0542702653	-2.0255249512
P39	-1.1952568738	-1.5675290732	0.9643914845
Cl40	-1.3377684296	2.8043575911	-0.9052124992
Pd41	-1.2679503565	0.5567086828	0.0621326323
O42	-0.9115541315	-1.7648329206	2.4404139877

2^1-Pt

E(SCF)= -2300.91542575912

P1	1.0486468111	0.2986277942	0.1234697022
P2	-3.5201187116	0.1846438720	-0.3292655046
C3	-3.8279563930	-1.6177009812	-0.1085125198
C4	-5.0668872292	-2.2046155739	-0.4013777762
C5	-2.7932152030	-2.4013718968	0.4378866543
C6	-5.2832449637	-3.5572463410	-0.1465130651
H7	-5.8714125666	-1.6060408934	-0.8215819966
C8	-3.0416325730	-3.7484769661	0.7378508399
C9	-4.2721258773	-4.3267360882	0.4333308626
H10	-6.2444518051	-4.0060851107	-0.3806693237
H11	-2.2780639135	-4.3379141618	1.2367515721
H12	-4.4487587442	-5.3746851307	0.6594223240
C13	1.2928885567	-1.4833085511	-0.2841048168
C14	2.4660727259	-1.9846703964	-0.8564836494
C15	0.2089866670	-2.3498999749	-0.0158341180
C16	2.5671779334	-3.3388254736	-1.1790484366
H17	3.3022972917	-1.3227277859	-1.0655753825
C18	0.3292054972	-3.7054053282	-0.3369120054
C19	1.4969055137	-4.1953671512	-0.9245503862
H20	3.4769469402	-3.7210620602	-1.6333660260

H21	-0.4941744893	-4.3854751286	-0.1445881914
H22	1.5697682255	-5.2480318514	-1.1840958993
C23	-4.7109934796	1.0315029998	0.7889877425
H24	-4.5752577957	2.1104453844	0.6732241466
H25	-5.7461111515	0.7638016649	0.5555819382
H26	-4.4874040016	0.7589466675	1.8229253086
C27	-4.0937808409	0.6233163048	-2.0177824555
H28	-5.1694463584	0.4626996474	-2.1371609486
H29	-3.8498495978	1.6761248024	-2.1832681583
H30	-3.5480816991	0.0231520200	-2.7491941772
C31	1.8526152860	0.5510588776	1.7586187808
H32	2.9082564307	0.2638861310	1.7361779771
H33	1.7640401489	1.6042435390	2.0397218984
H34	1.3164623288	-0.0599809791	2.4898159405
C35	2.0339713567	1.2762844603	-1.0745881091
H36	1.7842262106	2.3298909135	-0.9258763396
H37	3.1092976576	1.1253451929	-0.9422636224
H38	1.7403486802	1.0019053776	-2.0900831972
P39	-1.2004447604	-1.5937380240	0.9363955395
Cl40	-1.3141169857	2.7974671834	-0.8996997600
Pt41	-1.2664863220	0.5232545963	0.0394429968
O42	-0.9515335073	-1.8090098139	2.4159970330

3^3-V

E(SCF)= -2060.17845736913

C1	-3.5234577478	-1.5824353883	-0.2508064753
C2	-4.7562953270	-2.0217577390	-0.7636021830
C3	-2.7274626558	-2.4784747392	0.4868876091
C4	-5.1649810520	-3.3328573514	-0.5239098860
H5	-5.3848285938	-1.3609386214	-1.3484706574
C6	-3.1549729720	-3.7810393443	0.7360973765
C7	-4.3784861515	-4.2143861184	0.2224185821
H8	-6.1160009529	-3.6706019802	-0.9259868559
H9	-2.5467314291	-4.4532668453	1.3340283505
H10	-4.7189945005	-5.2286028937	0.4069592412
C11	1.0219776521	-1.5666756914	-0.2275812923
C12	2.2623616086	-1.9977203068	-0.7291868420
C13	0.2226538363	-2.4697389867	0.4979311070
C14	2.6744580325	-3.3081472782	-0.4915135162
H15	2.8939597432	-1.3312376761	-1.3043207234
C16	0.6532987148	-3.7716962336	0.7449243011
C17	1.8840401565	-4.1969467066	0.2419034136
H18	3.6311840403	-3.6396546721	-0.8851413006
H19	0.0417961559	-4.4496858673	1.3328854081

H20	2.2270112515	-5.2106282423	0.4247319617
C21	-3.9394340532	0.7273725414	-0.9105420551
H22	-4.8491368704	0.7223194006	-0.2997983472
H23	-3.4920876678	1.7197588474	-0.8404591189
H24	-4.1874590271	0.5484359987	-1.9640113501
C25	1.4319369580	0.7482968188	-0.8736800914
H26	0.9774902270	1.7375937943	-0.8056464766
H27	2.3345562169	0.7467277396	-0.2524400773
H28	1.6934329831	0.5742321453	-1.9247433101
P29	-1.2573233868	-1.6399602468	1.1130684922
Cl30	-1.2720943434	2.1292737683	0.9252795684
Cl31	-1.2430434619	0.8168644175	-2.5686191496
N32	-3.0061640103	-0.2914869765	-0.4119227820
N33	0.4993210685	-0.2779022183	-0.3893263084
O34	-1.2636552334	-1.3334918383	2.5881774774
V35	-1.2561857784	0.3766435028	-0.3693819844

4^3-V

E(SCF)= -2667.24460242826

C1	-3.4189520191	-2.0302069691	-0.5792695304
C2	-4.5426417537	-2.6605924006	-1.1280759411
C3	-2.7779054359	-2.5798568185	0.5318013114
C4	-5.0268081854	-3.8239357991	-0.5293214924
H5	-5.0398785466	-2.2356835116	-1.9944949673
C6	-3.2813036556	-3.7313869052	1.1449349524
C7	-4.4082487391	-4.3548401963	0.6070557752
H8	-5.9058392513	-4.3103409078	-0.9423385640
H9	-2.8030263183	-4.1230782785	2.0381298814
H10	-4.8088724051	-5.2481330673	1.0768347197
C11	1.1718110137	-1.7109374080	-0.0644952221
C12	2.3610730043	-2.2195453243	-0.5922934991
C13	0.1162193931	-2.5636957480	0.2858772584
C14	2.4773357724	-3.5978038303	-0.7805963287
H15	3.1734177404	-1.5521932456	-0.8614351794
C16	0.2415887307	-3.9397351067	0.0861987887
C17	1.4253265614	-4.4545697247	-0.4475109368
H18	3.3952446162	-4.0037684048	-1.1954703525
H19	-0.5765810560	-4.6058752697	0.3433188482
H20	1.5276075294	-5.5245372061	-0.6018086448
P21	-1.2891009194	-1.7097831475	1.0828627760
Cl22	-2.0126387220	1.7518854189	1.3667720682
Cl23	-0.9323130799	1.8357580572	-1.9529601908
O24	-1.1727247428	-1.5829861281	2.5775683460
S25	-2.8232826872	-0.4993702189	-1.2635650479

S26	0.9388260883	0.0394015507	0.1883825188
V27	-1.1811085973	0.5598996246	-0.1862663916

5^1-Ni

E(SCF)= -1777.71182433748

C1	-3.6577018492	-1.3775227916	-0.3025456966
C2	-4.8874050409	-1.7912363745	-0.8244464211
C3	-2.7677375297	-2.3219420467	0.2240995929
C4	-5.2182018503	-3.1459634551	-0.8282236020
H5	-5.5932243607	-1.0732016938	-1.2265738613
C6	-3.1253089787	-3.6758796021	0.2438805009
C7	-4.3405242002	-4.0912033427	-0.2950911366
H8	-6.1712886704	-3.4613135757	-1.2430377859
H9	-2.4527020886	-4.4063689719	0.6828927309
H10	-4.6062991240	-5.1444040326	-0.2946309285
C11	1.1262905197	-1.3603350235	-0.2704890883
C12	2.3638974655	-1.7656646491	-0.7798245110
C13	0.2323361383	-2.3122320892	0.2360269181
C14	2.6985357334	-3.1194612677	-0.7920375152
H15	3.0726668231	-1.0421074975	-1.1664669584
C16	0.5929126038	-3.6652964067	0.2466595536
C17	1.8163882198	-4.0721674548	-0.2801763044
H18	3.6578708346	-3.4282191405	-1.1973427477
H19	-0.0840050586	-4.4021622026	0.6680048140
H20	2.0848107792	-5.1246714784	-0.2871436450
C21	-3.9530324764	0.7040676702	0.9263832353
H22	-3.6262561591	1.7441949084	0.9654054035
H23	-5.0438335345	0.6490186028	0.8174258327
H24	-3.6520839355	0.1920239556	1.8419389311
C25	-3.6699514191	0.7588236434	-1.5013549869
H26	-4.7598425646	0.8037700376	-1.6066071846
H27	-3.2635485654	1.7679859979	-1.4614476279
H28	-3.2456314276	0.2254903891	-2.3541597135
C29	1.3859599410	0.7106330975	0.9855680255
H30	2.4791608503	0.6609615399	0.9004714898
H31	1.0544881245	1.7492358916	1.0267357093
H32	1.0666903164	0.1893398061	1.8896310779
C33	1.1567820041	0.7885300644	-1.4466786659
H34	0.7437857174	1.7949270741	-1.4061745486
H35	2.2485538874	0.8404691606	-1.5261003552
H36	0.7552196343	0.2617851330	-2.3144449129
P37	-1.2731313590	-1.5822611556	0.9794279861
Cl38	-1.2793578066	2.6499929850	-0.2674206470
Ni39	-1.2723790839	0.3226798345	-0.0172325395

O40	-1.2786189404	-1.6905802143	2.4914472792
N41	-3.2809214552	0.0527960888	-0.2431439949
N42	0.7428930845	0.0679022505	-0.2049350199

6^1-Ni

E(SCF)= -2384.79545313567

C1	-3.7713245061	-1.5673517589	-0.2675899181
C2	-5.0017690501	-2.0823404760	-0.6889716934
C3	-2.8122031365	-2.3908411139	0.3345841492
C4	-5.2706535524	-3.4392250648	-0.5179455541
H5	-5.7505423517	-1.4300810978	-1.1286815314
C6	-3.1258552234	-3.7409429497	0.5557605407
C7	-4.3376559129	-4.2675047628	0.1129807072
H8	-6.2221287405	-3.8440415120	-0.8502784224
H9	-2.4251601220	-4.3737989885	1.0922848286
H10	-4.5643235129	-5.3173914119	0.2735407153
C11	1.2120003581	-1.4318763150	-0.1946517799
C12	2.4105010491	-1.8724632251	-0.7586814898
C13	0.1484828942	-2.3201799310	0.0378488352
C14	2.5397602086	-3.2116275383	-1.1304346432
H15	3.2375863884	-1.1869952920	-0.9127554098
C16	0.3053914901	-3.6622861174	-0.3275489979
C17	1.4882124809	-4.1042626022	-0.9211109116
H18	3.4654421756	-3.5549119472	-1.5831749135
H19	-0.5064680807	-4.3640128920	-0.1671831837
H20	1.5891846986	-5.1439113027	-1.2188365379
C21	-3.5230981880	0.5204569081	-2.1557500793
H22	-4.5541946505	0.4069684498	-2.4947755076
H23	-3.1836104894	1.5490972604	-2.2805482128
H24	-2.8609043326	-0.1654077897	-2.6845149269
C25	1.6849478183	1.2041204587	-1.1062668631
H26	1.3013294944	2.2204164302	-1.0144129644
H27	2.7737165559	1.1905893354	-1.0346587674
H28	1.3439612218	0.7664819328	-2.0444019521
P29	-1.2765620745	-1.5966478867	0.9706764518
Cl30	-1.3088634648	2.6109361319	-0.5797566677
Ni31	-1.2774413761	0.4450869546	0.1152429650
O32	-1.1226473669	-1.8163756278	2.4589035836
S33	-3.4503336445	0.2099357221	-0.3482198534
S34	0.9796174799	0.2915559409	0.3147213201

7^1-Ni

E(SCF)= -2539.21593623750

C1	-3.3103131475	-1.7233762590	-0.2980513892
C2	-3.6819109046	-0.3996096985	0.0571500143
C3	-4.9526487917	0.0682640029	-0.3018154425
C4	-5.8685726749	-0.7361505207	-0.9767474501
C5	-5.5059605160	-2.0389616998	-1.3078155216
C6	-4.2432523753	-2.5243325573	-0.9795786138
P7	-2.5443204682	0.6683261527	1.0255399154
C8	1.7446846041	-2.6947186218	0.4875491203
C9	2.4070315649	-3.9182648195	0.7479090129
C10	3.7886488106	-4.0010817969	0.8553151612
C11	4.5795725645	-2.8624329254	0.7136772837
C12	3.9461532667	-1.6424451460	0.5134047052
C13	2.5496541047	-1.5166772938	0.4215891376
P14	1.8573780384	0.1796957314	0.3610438487
H15	5.6615812341	-2.9176428724	0.7775529041
H16	4.2453872120	-4.9685696523	1.0450711241
H17	4.5595481410	-0.7502918099	0.4383371142
H18	1.8332538187	-4.8281808991	0.8617328652
H19	-6.2026404546	-2.6840707153	-1.8361531709
H20	-3.9759661849	-3.5330601797	-1.2705246159
H21	-6.8491656573	-0.3486880749	-1.2355530560
H22	-5.2442796698	1.0799550455	-0.0395165218
N23	0.3597264318	-2.6904931205	0.3166007654
N24	-2.0499147252	-2.2353051296	0.0685464000
P25	-0.5776882919	-1.3741734772	-0.3564317949
C26	-1.8009854768	-3.6716475483	-0.0637581219
H27	-1.7943579888	-3.9919274132	-1.1167963440
H28	-2.5749045883	-4.2395556417	0.4620318788
C29	-0.4261669431	-3.9046700750	0.5637501152
H30	0.0335121044	-4.7802068623	0.0944416189
H31	-0.5050618965	-4.0951600024	1.6430304190
Ni32	-0.3248746558	0.3972239026	0.8501886501
O33	-0.3723101616	-1.2110404525	-1.8414764176
C34	2.1374873280	0.8073741568	-1.3491245538
H35	3.1871366730	0.6959815823	-1.6377041312
H36	1.4921939961	0.2471120049	-2.0295556117
H37	1.8625513457	1.8660563436	-1.3792578957
C38	3.0018169998	1.1892715263	1.3922135586
H39	3.9990084844	1.2455413998	0.9479742100
H40	2.5743332013	2.1893683362	1.4769032778
H41	3.0663614498	0.7626209421	2.3952101621
C42	-3.0374413312	2.3889276459	0.5941378792
H43	-2.9409746567	2.5366883039	-0.4844371248
H44	-4.0626935930	2.6113043661	0.9024986957

H45	-2.3460266485	3.0566265324	1.1106952561
C46	-3.0988793073	0.4477842748	2.7701919145
H47	-2.4973503514	1.1052977314	3.4018439274
H48	-4.1622611373	0.6837743114	2.8730224771
H49	-2.9292633195	-0.5892611934	3.0705200553
Cl50	-0.0371784727	2.2065406662	2.1990870320

4^3-V Transition state

E(SCF)= -2825.71741590203

C1	-3.3396378011	-2.0818429168	-0.6749611866
C2	-4.4524122828	-2.7292118534	-1.2257527087
C3	-2.7156013615	-2.6247813339	0.4618771823
C4	-4.9487507018	-3.8887943578	-0.6300914461
H5	-4.9325501250	-2.3154495486	-2.1070336598
C6	-3.2307893070	-3.7782064488	1.0606389567
C7	-4.3469243392	-4.4131202448	0.5151095205
H8	-5.8192496652	-4.3779662019	-1.0577278152
H9	-2.7684178323	-4.1766569673	1.9588993362
H10	-4.7461554216	-5.3081834605	0.9826500483
C11	1.1802396323	-1.6633735034	-0.1656003869
C12	2.4170156965	-2.1918675768	-0.5644852740
C13	0.2323458345	-2.5133379995	0.4340562924
C14	2.6920048789	-3.5452989579	-0.3811663210
H15	3.1515123181	-1.5408314044	-1.0280962391
C16	0.5112705845	-3.8768594623	0.5926282569
C17	1.7394712610	-4.3961899547	0.1867541793
H18	3.6526240945	-3.9418520463	-0.6975257565
H19	-0.2375213918	-4.5368566582	1.0223416871
H20	1.9502109503	-5.4546978003	0.3054516375
P21	-1.2693088096	-1.6954940754	1.0463042947
Cl22	-2.0340697503	1.4426324216	1.7282285869
Cl23	-1.2511832467	2.2514686875	-1.5605494234
O24	-1.2277025413	-1.6778786825	2.6432578490
S25	-2.7507913597	-0.5813196423	-1.4571467373
S26	0.8388658756	0.0518416438	-0.5205255195
V27	-1.3376025067	0.5640461453	-0.1251309922
H28	-1.0090955994	-2.7409141991	3.3107352838
C29	-0.8173183924	-3.7016378668	4.1538093250
H30	-1.1128975685	-4.5895798065	3.5816589097
C31	0.6732554745	-3.6864529937	4.4505176598
H32	0.8804077044	-4.5415194628	5.1178068774
H33	1.2220988965	-3.8945646514	3.5243126910
C34	-1.7821763277	-3.3818952794	5.2759842401

H35	-1.6800176676	-4.1238146016	6.0830765217
H36	-1.5920033921	-2.3961618557	5.7095254279
H37	-2.8202231341	-3.4067924981	4.9326376156
C38	1.2045113128	-2.3982419412	5.0902048260
H39	0.9888162412	-1.5316002822	4.4576639016
H40	0.7609247532	-2.2173951108	6.0742178880
H41	2.2889323180	-2.4580777945	5.2243564301

Mn porphyrin complex Transition state for breaking *n*-butane C-H bonds

E(SCF)= -1401.57903765082

Mn1	-0.2313538702	-0.0972677194	-0.0886458859
O2	0.3231486356	-1.6123154243	0.0986295725
N3	-1.8878675966	-0.8055350081	-1.0801766517
N4	0.7470751652	0.0547380935	-1.8921428425
N5	1.3879006730	0.6975787208	0.8783089157
N6	-1.2364622253	-0.1659858987	1.6889660407
C7	-0.9968084023	-0.8391058735	-3.3610565773
C8	2.8602139094	0.9805937683	-1.0663973195
C9	0.5414736873	0.6293097566	3.1759761376
C10	-3.3726803116	-1.0447582943	0.8538266865
C11	0.2744003402	-0.3221569773	-3.1116315241
C12	2.0180677665	0.5075088269	-2.0729569584
C13	2.5669910864	1.0588816665	0.2955221917
C14	1.5250580842	0.8891989036	2.2211965288
C15	-0.7406096885	0.1405513323	2.9215171369
C16	-2.5163573807	-0.6043261027	1.8640563430
C17	-3.0755680539	-1.1413686112	-0.5057931826
C18	-1.9974390640	-1.0552528249	-2.4135544044
C19	-3.3204768779	-1.5766373711	-2.7066275662
C20	-3.9908727000	-1.6279764662	-1.5225552075
H21	-3.6723358644	-1.8591104336	-3.6918644810
H22	-5.0048795520	-1.9622313108	-1.3373824819
C23	-2.8566326266	-0.5621886510	3.2728396821
C24	-1.7536677423	-0.1033192547	3.9295606645
H25	-3.8142039444	-0.8522930673	3.6888054343
H26	-1.6240747161	0.0611640148	4.9923635273
C27	2.3754508869	0.4171799974	-3.4773285050
C28	1.2931724181	-0.0996090765	-4.1217020982
H29	3.3310951531	0.7103745328	-3.8956593520
H30	1.1785408000	-0.3159569029	-5.1770424962
C31	2.8474302367	1.4105702049	2.5082088048
C32	3.4926572904	1.5180987228	1.3129933942
H33	3.2176372315	1.6559985537	3.4965538625

H34	4.5007118220	1.8669457826	1.1223068338
H35	0.7949006594	0.8323132033	4.2132166568
H36	3.8515666591	1.3070756301	-1.3714396627
H37	-1.2321839495	-1.0915294657	-4.3921709396
H38	-4.3681165327	-1.3571186570	1.1604254343
O39	-0.8927628836	1.5636415607	-0.4454795801
H40	-0.9409040996	2.3726919516	0.4069010681
C41	-0.9627598611	3.4492513139	1.2055521539
H42	-0.1080180431	3.2700927208	1.8651497183
C43	-0.7246242405	4.5859462204	0.2257891614
H44	-1.5780486827	4.6483941798	-0.4636938175
H45	0.1473031189	4.3415290637	-0.3923989137
C46	-2.2898505547	3.4530354472	1.9370137901
H47	-3.1274199857	3.4855339017	1.2286522008
H48	-2.4079213625	2.5576951958	2.5543491995
H49	-2.3953108177	4.3266160095	2.6029118341
C50	-0.5074723390	5.9587446508	0.8899263749
H51	-0.3284636564	6.7425345664	0.1425302335
H52	-1.3771736751	6.2631469289	1.4843986530