A Comparative Study on Hydrogenation of Ketone Catalyzed by Diphosphine-diamine Transitional Metal Complexes using DFT Method

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Abbreviations used in manuscript

TM : Transition metal

HT : Hydrogen transfer

DA : Dihydrogen activation

MHNH : *Trans*-dihydrido(diamine-diphosphine) metals complex

RH : The adduct of MHNH and acetone

MN: Hydridoamido complex produced after MHNH transferd the hydride and proton to acetone

PH : The adduct of MN and *i*-propanol

TSH: The transition state of HT

MN-H_2 : The adduct of H_2 and MN

TS： Transition state of DA

ZPE: Zero-point energy

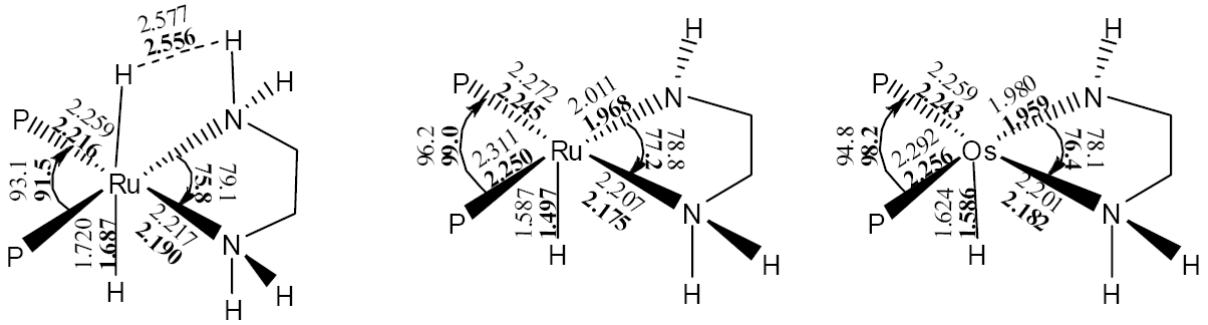
GI, GII, GIII: Group I, II and III

FMO: Frontier molecular orbital

DFT: Density functional theory

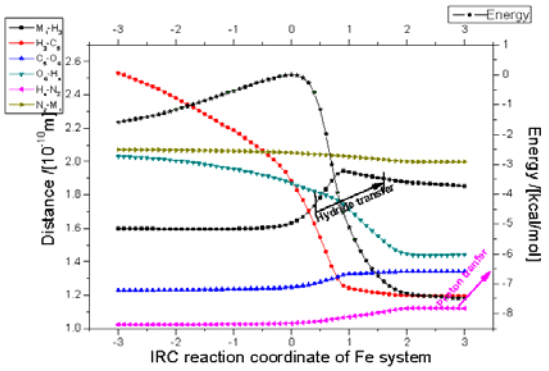
Supplemental figure and table legend:

Figure S1. A comparison between calculated structure and crystal structure. **(Plain text is calculated structure; bold text is the crystal structure.)**

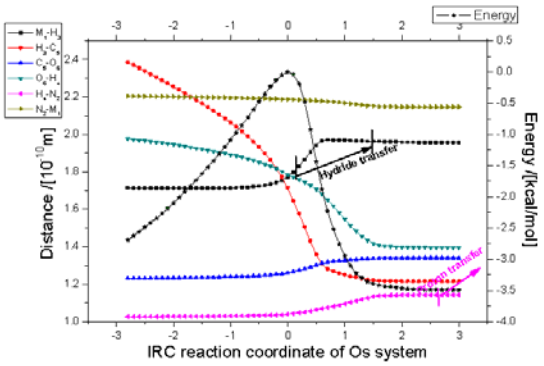


Calculated structures of RuHNH, RuN and OsN are very close to the crystal structures found by Morris' group (Abdur-Rashid, K.; Clapham, S. E.; Hadzovic, A.; Harvey, J. N.; Lough, A. J.; Morris, R. H., Mechanism of the Hydrogenation of Ketones Catalyzed by trans-Dihydrido(diamine)ruthenium(II) Complexes. *J. Am. Chem. Soc.* 2002, **124**, (50), 15104-15118; Sean E. Clapham and Robert H. Morris. Reactions of an Amido Hydrido Complex of Osmium, OsH(NHCMe2CMe2NH2)(PPh3)2: HX Addition, HX Transfer, and Ketone H2-Hydrogenation. *Organometallics* 2005, **24**, 479-481).

Figure S2. Structural changes along IRC pathway in HT (A, B, C, D, E) and DA (F, G, H) step for Fe, Co, Os, Ir and Pt systems.



A



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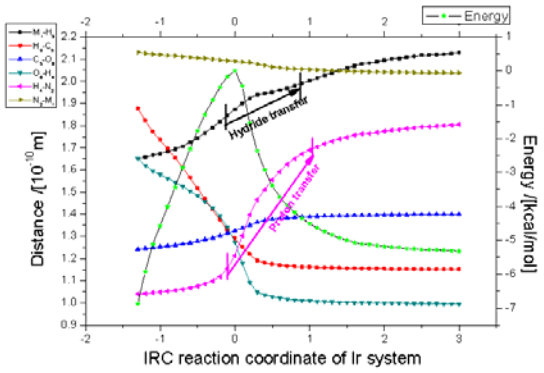
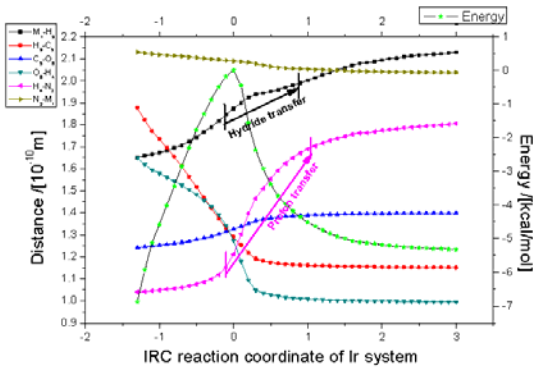
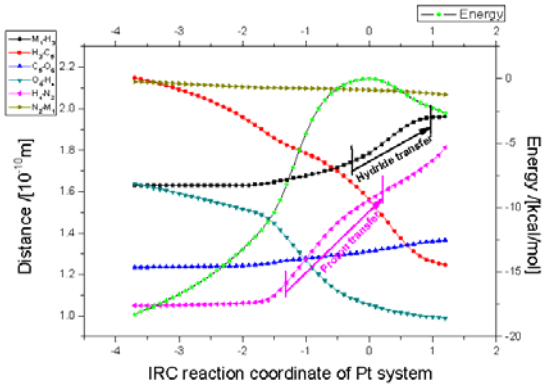


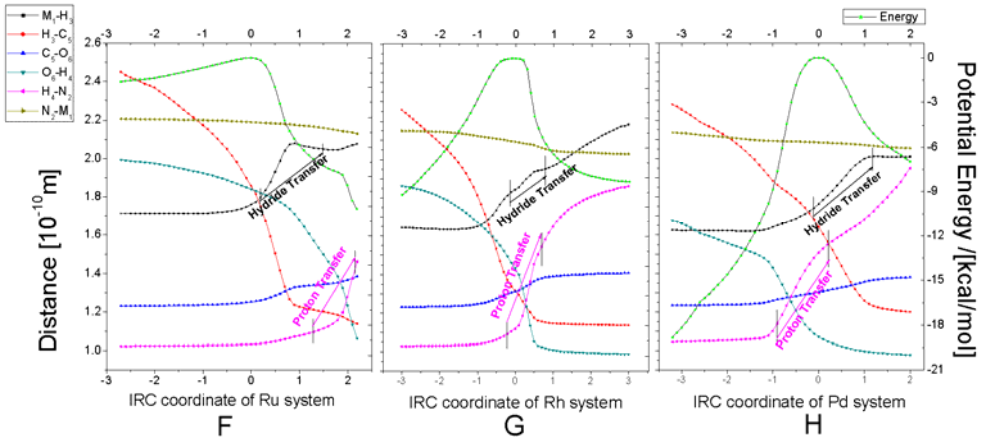
C



D

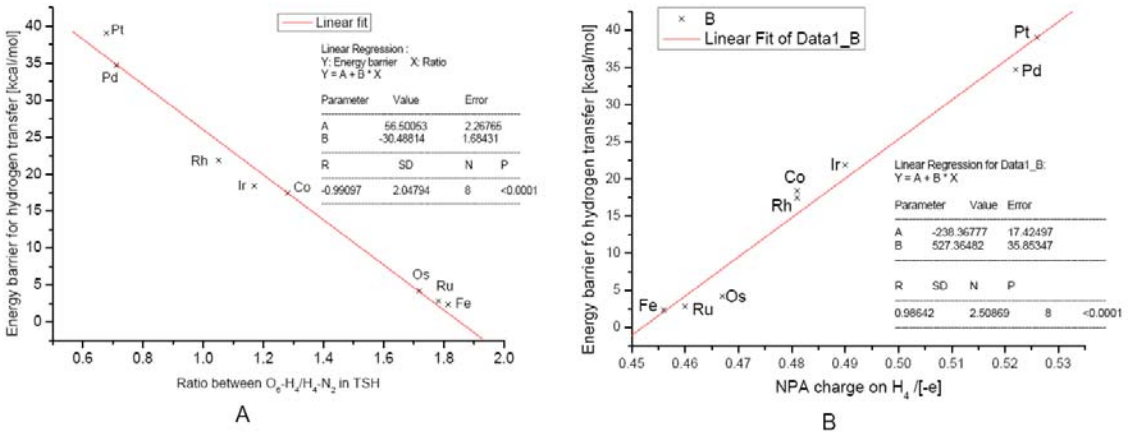


E



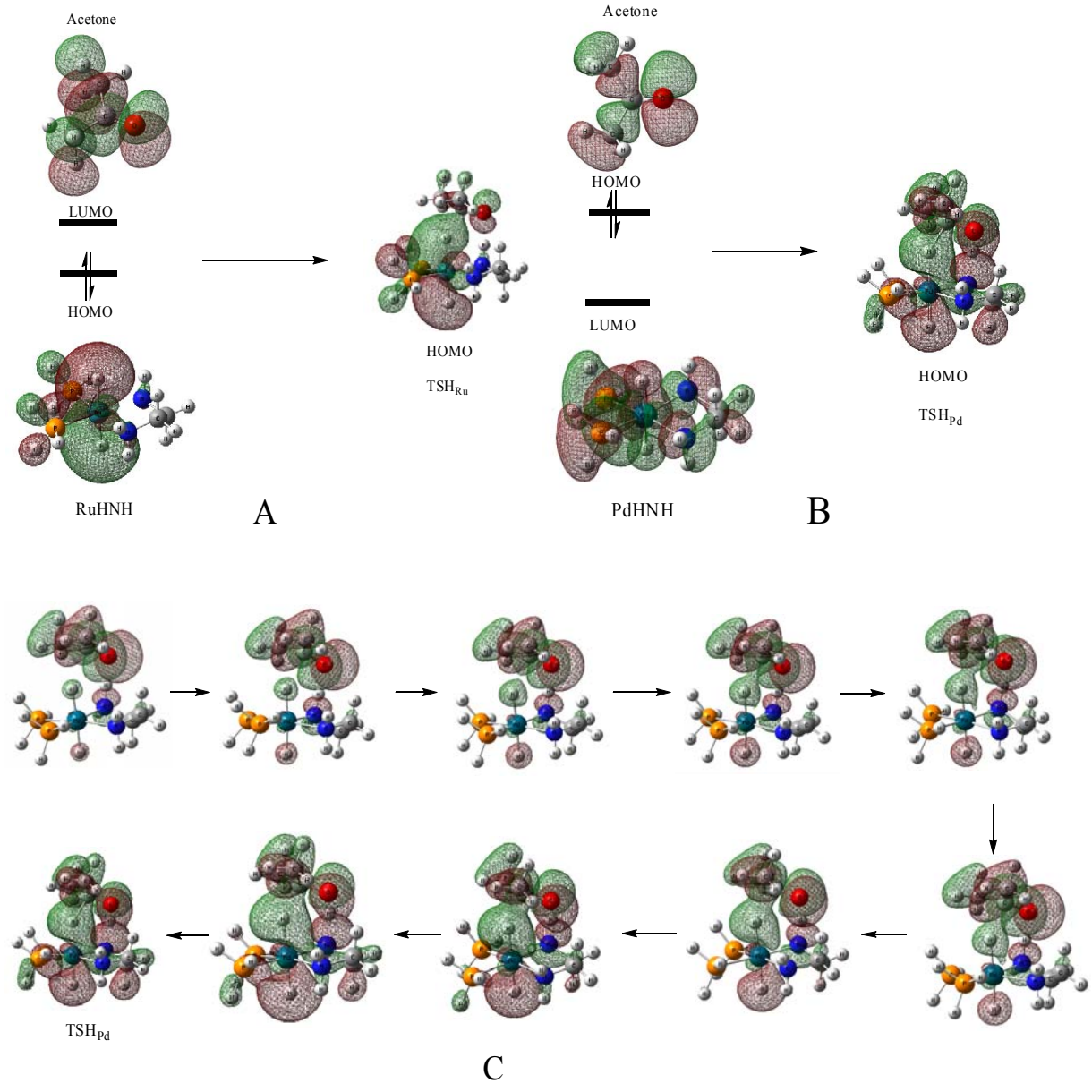
Three transfer modes are observed clearly through the structural changes along IRC pathways of Fe, Os, Co, Ir and Pt systems in hydrogen transfer step. Hydride transfers to carbonyl group before proton transfer for GI (A, B). Because the hydride transfers much early than proton transfer, it looks like a stepwise reaction (Y. Chen, S. Liu, M. Lei, *J. Phys. Chem. C*, 2008, **112**, 13524) in GI. For GII hydride transfer and proton transfer occur simultaneously (C, D); for GIII, proton transfers to carbonyl preceding hydride transfer (E). In dihydrogen activation step, GI, GII and GIII display similar action from the comparison among F, G and H.

Figure S3. Relationships between energy barriers and structures.



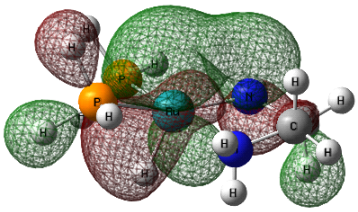
The energy barriers of hydrogen transfer for the eight complexes have a good linear relationship with the substructure N_2-H_4-O_6 in TSH (A) and with the NPA charge on H_4 in TSH (B). In TSH, the larger the ratio of O_6-H_4/H_4-N_2 is, the higher energy barrier is. For example, it is obvious that proton transfers to oxygen of carbonyl in TSH_{Pd} and TSH_{Pt}. Therefore they have large ratio of O_6-H_4/H_4-N_2 which corresponds to a high energy barrier. These relationships agree with the three hydrogen transfer modes.

Figure S4. The interaction between frontier molecular orbital (FMO) of MHNH and that of acetone.

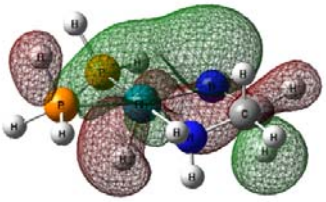


In hydrogenation transfer step, the interactions between frontier molecular orbitals are different each other for three groups. For GI, LUMO of acetone matches HOMO of RuHNH well (A). The most extended part of RuHNH is placed on the hydride which is located in the front of the extended carbon atom on carbonyl. For GIII, LUMO does not extend on hydride and proton in PdHNH (B). We describe the change of HOMO along IRC pathway (C) to understand the interaction between the two molecular orbitals (MOs). With the approaching of two molecules, part of MO on hydride and proton extends gradually to match the acetone moiety. The structure changes during this induction process. The proton on PdHNH moiety is transferred to oxygen of carbonyl moiety.

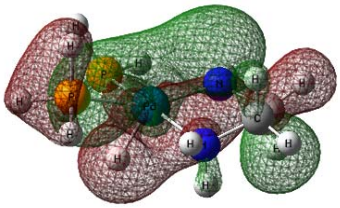
Figure S5. The HOMO of RuN, RhN and PdN.



HOMO of RuN



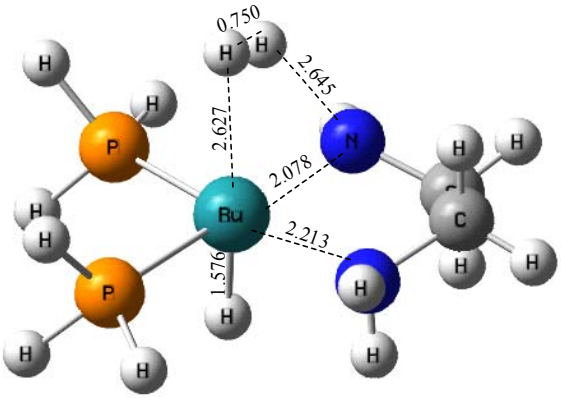
HOMO of RhN



HOMO of PdN

The delocalization effect becomes stronger from GI to GIII according to the HOMO above of RuN, RhN, and PdN.

Figure S6. The transition state for dihydrogen coordination.



Dihydrogen coordinated at the vacant site of MN to form η^2-H_2 complex (MN-H_2). This process may go via a transition state because the potential energy of MN-H_2 is higher than the sum of MN and H_2. However, only the transition state for Ru system was located and confirmed by only one imaginary frequency (215.3 *i*). The energy barrier for this coordination step was only 1.4 kcal/mol. This barrier disappeared if zero-point energy (ZPE) was included. Its Cartesian coordinates were shown as the following:

Energy: -971.938638718 a.u.

	X	Y	Z
Ru	0.006745	-0.150974	0.022142
P	0.002138	0.042470	2.335267
N	2.211764	-0.165549	-0.164237
P	-2.242695	-0.412914	-0.181452
N	0.228013	-0.142820	-2.044116
C	1.558549	-0.551828	-2.473351
C	2.569032	0.151522	-1.577833
H	-0.465539	-0.650845	-2.590461
H	2.479412	-1.124654	0.050354
H	-0.727650	-0.856783	3.163225
H	1.233919	-0.113892	3.039929
H	-3.185224	0.632301	0.037964
H	-2.936305	-1.396498	0.571467
H	1.743286	-1.645233	-2.407350
H	1.760920	-0.265858	-3.519995
H	3.602617	-0.142503	-1.805005
H	2.472201	1.234917	-1.700878
H	0.065338	-1.712581	0.227970
H	-0.390875	1.209303	3.062699
H	-2.738867	-0.796801	-1.457657
H	2.720403	0.433861	0.482479

H	-0.079828	2.472203	-0.098479
H	-0.088087	2.158022	-0.779314

Figure S7. Geometrical structures in the whole catalytic cycles for all systems.

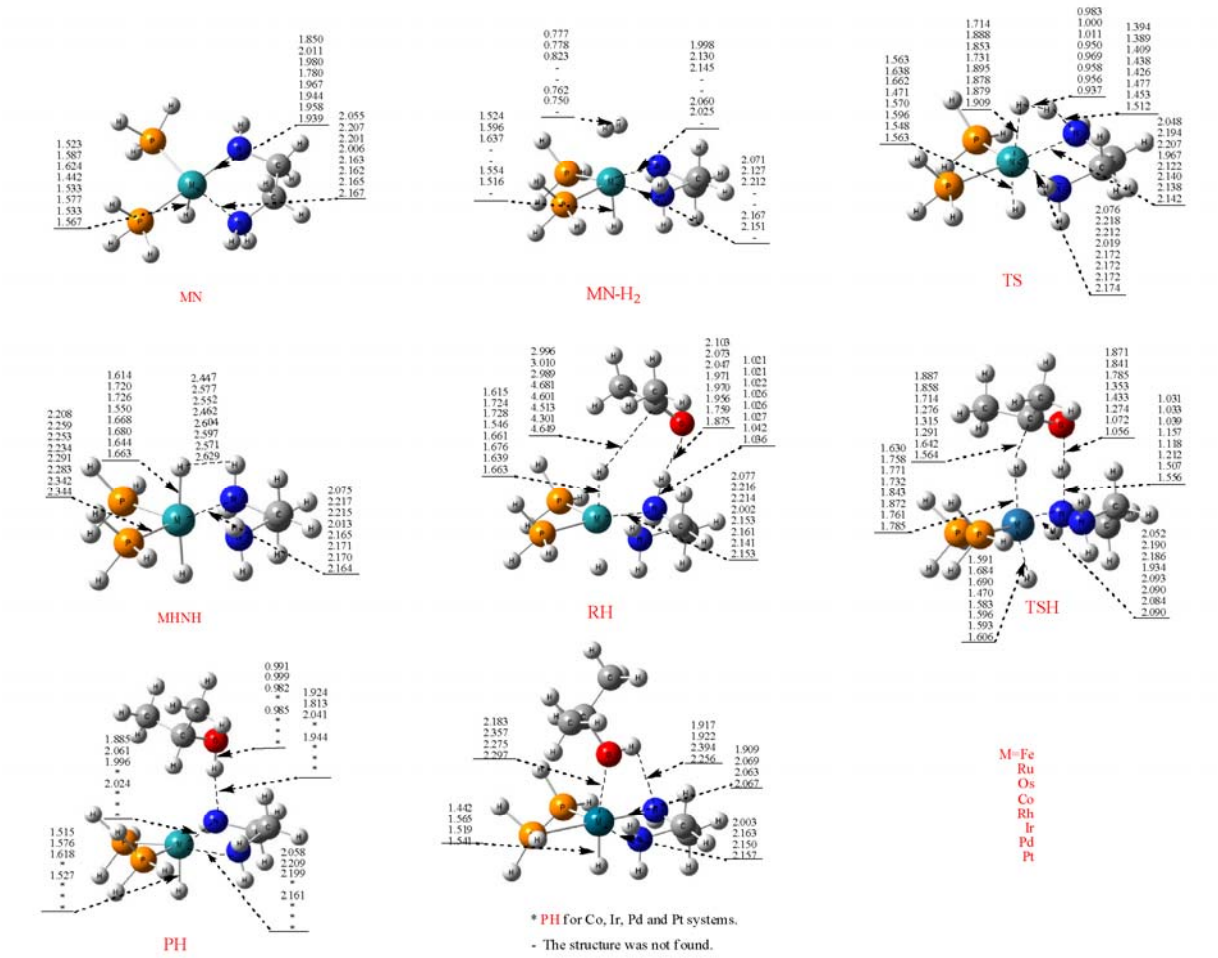


Table S1. Structural parameters [a] and charges distribution [b] of MHNH

	M_1-P_7	M_1-P_8	M_1-N_9	M_1-N_2	M_1-H_3	M_1-H_{10}	N_2-H_4	P_7-M_1-P_8	N_2-M_1-N_9	P_7-P_8-N_9-N_2	M_1	H_3	N_2	H_4
Fe	2.208	2.208	2.075	2.075	1.614	1.614	1.017	93.3	82.3	4.2	-0.056	-0.373	-0.848	0.434
Ru	2.259	2.259	2.217	2.217	1.720	1.720	1.017	93.1	79.1	1.5	-0.406	-0.304	-0.845	0.435
Os	2.253	2.253	2.215	2.215	1.726	1.726	1.017	93.0	78.6	1.6	-0.351	-0.313	-0.859	0.44
Co	2.234	2.2337	2.013	2.013	1.550	1.550	1.019	91.3	84.4	4.6	0.332	-0.295	-852	0.451
Rh	2.291	2.291	2.165	2.165	1.668	1.668	1.019	92.1	80.8	1.1	0.076	-0.262	-0.847	0.45
Ir	2.283	2.283	2.171	2.171	1.680	1.680	1.019	92.5	80.0	0.6	0.094	-0.274	-0.863	0.455
Pd	2.342	2.342	2.170	2.170	1.644	1.644	1.021	92.6	81.3	18.0	0.545	-0.184	-867	0.471
Pt	2.344	2.344	2.164	2.164	1.663	1.663	1.022	92.0	80.6	-1.2	0.587	-0.235	-0.87	0.473

a: unit for bond length: angstrom (Å), for angle: degree (˚); b: NPA charge, unit: e.

Table S2. Structural parameters [a] and charge distribution [b].

	M_1-H_3	H_3-C_5	C_5-O_6	O_6-H_4	H_4-N_2	N_2-M_1	O_6-H_4/H_4-N_2	M_1	H_3	C_5	O_6	H_4	N_2
Fe	1.630	1.887	1.248	1.871	1.031	2.052	1.814	-0.035	-0.278	0.524	-0.697	0.456	-0.853
Ru	1.758	1.858	1.251	1.841	1.033	2.190	1.782	-0.368	-0.237	0.517	-0.707	0.46	-0.852
Os	1.771	1.714	1.260	1.785	1.039	2.186	1.718	-0.313	-0.214	0.48	-0.723	0.467	-0.874
Co	1.732	1.276	1.320	1.353	1.157	1.934	1.169	0.377	-0.022	0.237	-0.775	0.481	-0.857
Rh	1.843	1.315	1.310	1.433	1.118	2.093	1.2811	0.13	-0.033	0.264	-0.773	0.481	-0.85
Ir	1.872	1.291	1.325	1.274	1.212	2.090	1.052	0.15	-0.028	0.26	-0.785	0.49	-0.9
Pd	1.761	1.642	1.303	1.072	1.507	2.084	0.712	0.595	-0.185	0.489	-0.691	0.522	-0.821
Pt	1.785	1.564	1.311	1.056	1.556	2.090	0.678	0.62	-0.168	0.458	-0.701	0.526	-0.881

a: unit for bond length: angstrom (Å), for angle: degree (˚); b: NPA charge, unit: e.

Table S3. Calculated energies and structures using LANL2DZ basis set and modified LANL2DZ basis set for Ru.

A: Comparison of energy of the whole catalytic cycle. (Unit: kcal/mol)

	RuHNH+Acetone+H_2	RH+H_2	TSH+H_2	PH+H_2	MN+H_2+Propanol	MN-H_2+Propanol	TS+Propanol	MHNH+Propanol
B3LYP/BSI	0	-5.26	-2.41	-14.98	-7.37	-6.26	5.11	-16.57
B3LYP/BSII	0	-5.24	-2.07	-13.94	-6.69	-5.84	5.25	-16.57

B: Comparison of the structure. (Unit: Å for bond length and ° for angle)

RuHNH									
	M1-P7	M1-P8	M1-N9	M1-N2	M1-H3	M1-H10	N2-H4	P7-M1-P8	N2-M1-N9
B3LYP/BSI	2.259	2.259	2.217	2.217	1.720	1.720	1.017	93.1	79.1
B3LYP/BSII	2.259	2.259	2.222	2.222	1.718	1.718	1.017	93.1	79.0
RuN									
	M1-P7	M1-P8	M1-N9	M1-N2	M1-H10	P7-M1-P8	N2-M1-N9		
B3LYP/BSI	2.272	2.311	2.207	2.011	1.587	96.2	78.8		
B3LYP/BSII	2.271	2.306	2.209	2.012	1.591	96.1	78.6		

BSI=LANL2DZ for Ru and 6-31+G** gor other atoms.

BSII=LANL2DZ + p (*J. Comput. Chem. 1996, 11, 1359)* for Ru and 6-31+G** for other atoms.

From two tables above, we can see that the results calculated using two basis set have little differences. Therefore, (n+1) *p*-orbital does not affect the result dramatically and BS1 is suitable and economic to describe these systems.

Table S4. The calculated M1-N2 bond lengths[a] in MN and energy barriers[b] of DA using three different DFT functionals.

	B3LYP/BSI		PBEPBE/BSI		mPW1PW91/BSI	
	M_1-N_2	E_{DA}	M_1-N_2	E_{DA}	M_1-N_2	E_{DA}
Ru	2.011	12.48	2.000	7.75	1.993	7.68
Os	1.980	15.28	1.973	10.05	1.963	9.98
Rh	1.9670	15.20	1.963	9.87	1.950	10.99
Ir	1.944	16.61	1.942	11.72	1.926	12.01
Pd	1.958	16.03	1.958	10.92	1.934	12.30
Pt	1.939	17.34	1.943	12.76	1.9178	13.56

a: Unit: angstrom (Å); b: Unit: kcal/mol.

Table S5. The calculated energies of the stationary points in DA process using modified LANL2DZ basis set for Ru.

	RuN[a]	TS_{Ru}[a]	RuHNH[a]	H_2[a]	E_{DA}[b]
B3LYP/BSII[c]	-970.772	-971.931	-971.966	-1.17854	11.94
mPW1PW91/BSII[c]	-970.742	-971.904	-971.94	-1.17342	7.05

a: Unit: a.u.; b: Unit: kcal/mol; c: BSI= LANL2DZ + p basis set (J. Comput. Chem. 1996, 11, 1359) for Ru and 6-31+G** basis set for other atoms.

Table S6. Imaginary frequencies of TSHs and TSs (unit: *i*).

	Fe	Ru	Os	Co	Rh	Ir	Pd	Pt
ν_{TSH}	177.8	224.9	261.4	457.9	185.6	886.3	695.5	607.2
ν_{TS}	1142.7	1301.9	1289.9	1213.9	1349.3	1240.8	1422.6	1280.8

The energies, and Cartesian coordinates of all the stationary points optimized for eight systems.

Results of TS, MN and MHNH calculated using B3LYP/BSI

FeN -1000.26848012 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Fe	-0.156014	-0.018042	0.124326
P	-1.510474	1.708754	-0.229593
N	1.494319	1.153517	0.482642
P	-1.742407	-1.562476	0.031063
N	1.143891	-1.261676	-0.308638
C	2.547421	-0.920834	-0.130642
C	2.645686	0.593461	-0.270047
H	1.024317	-2.270356	-0.356366
H	1.627143	1.021937	1.484889
H	-2.773781	1.821493	0.412311
H	-1.048471	3.002679	0.151888
H	-2.630091	-1.769549	-1.065763
H	-2.739877	-1.614535	1.036182
H	2.934515	-1.218736	0.864249
H	3.201487	-1.399902	-0.876746
H	3.607185	0.987281	0.087505
H	2.512140	0.876209	-1.319030
H	-0.581022	0.204832	1.569383
H	-1.985434	2.118246	-1.513494
H	-1.328410	-2.918208	0.130635
H	1.403763	2.154890	0.325926

RuN -970.764125442 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.001100	-0.005840	0.004836
P	-0.000011	-0.007744	2.315582
N	2.199050	0.001803	-0.191931
P	-2.254239	-0.137498	-0.240086
N	0.222134	0.654596	-1.881230
C	1.553171	0.581473	-2.466670
C	2.561093	0.857424	-1.357203
H	-0.494943	0.589798	-2.599936
H	2.442611	-0.969713	-0.380051
H	-0.480848	-1.062902	3.146562
H	1.259375	0.100518	2.979896
H	-3.182900	0.662118	0.485982
H	-2.939638	-1.365928	-0.049860
H	1.777481	-0.407316	-2.915337

H	1.696792	1.326107	-3.266500
H	3.593986	0.677784	-1.685774
H	2.465724	1.897742	-1.031246
H	0.022624	-1.579418	0.207609
H	-0.628067	1.028516	3.067444
H	-2.788477	0.151897	-1.527413
H	2.715284	0.281818	0.639355

OsN -967.943467660 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	0.000668	-0.003858	0.000878
P	0.000635	-0.005404	2.292444
N	2.194304	0.004968	-0.182220
P	-2.250017	-0.033627	-0.189337
N	0.261577	0.891294	-1.745978
C	1.592856	0.972438	-2.337985
C	2.599771	1.026746	-1.193797
H	-0.468363	1.075143	-2.428176
H	2.453812	-0.928426	-0.501222
H	-0.273403	-1.103227	3.171028
H	1.231879	0.346798	2.928774
H	-3.118255	0.605511	0.743158
H	-2.971253	-1.257763	-0.255419
H	1.817149	0.103522	-2.984701
H	1.712561	1.871667	-2.960413
H	3.628447	0.862041	-1.539574
H	2.538474	2.000475	-0.699500
H	0.002161	-1.608536	0.250886
H	-0.805649	0.926045	3.008395
H	-2.828617	0.551770	-1.355935
H	2.683314	0.161718	0.697021

CoN -1021.71788554 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Co	0.001308	-0.009437	-0.001077
P	0.000758	-0.008137	2.253039
N	1.801160	0.005829	-0.002609
P	-2.201369	-0.731515	-0.137185
N	0.195670	0.203579	-1.986486
C	1.578930	-0.229586	-2.361353
C	2.483403	0.298715	-1.263562
H	-0.493260	-0.271367	-2.567924
H	-0.120915	-1.234845	2.940828
H	1.168213	0.497605	2.857349
H	-3.136680	-0.254314	0.803874
H	-2.507546	-2.110162	-0.075329
H	1.587086	-1.322781	-2.365032
H	1.850748	0.135579	-3.356841
H	3.463102	-0.195068	-1.298445
H	2.660814	1.378655	-1.394075
H	-0.574588	1.308614	0.105122
H	-0.980219	0.747012	2.924506

H	-2.902340	-0.404158	-1.317973
H	2.371637	0.300079	0.786559
H	0.084269	1.201141	-2.174965

RhN -986.188850383 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Rh	-0.003828	-0.001541	-0.000981
P	0.000129	-0.004731	2.314681
N	1.963284	0.008330	-0.010357
P	-2.311842	-0.633653	-0.207422
N	0.331810	0.209046	-2.126909
C	1.754681	-0.182503	-2.397145
C	2.598060	0.392949	-1.273949
H	-0.301324	-0.315821	-2.728771
H	-0.356273	-1.190428	2.989971
H	1.247989	0.257829	2.913812
H	-2.906140	-0.469812	-1.477759
H	-3.302241	0.002231	0.570188
H	1.798245	-1.274699	-2.375720
H	2.072464	0.170422	-3.383808
H	3.615318	-0.017853	-1.324341
H	2.685851	1.486320	-1.386085
H	-0.594376	1.410977	0.070551
H	-0.814282	0.923342	2.991298
H	-2.676071	-1.977845	0.030165
H	2.504114	0.352948	0.780101
H	0.194505	1.193622	-2.358411

IrN -981.412463795 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ir	-0.000942	-0.002004	0.003530
P	-0.000290	-0.003106	2.347945
N	2.152132	0.000515	-0.195717
P	-2.288080	-0.075734	-0.197310
N	0.188062	0.811559	-1.751584
C	1.512764	0.873906	-2.377064
C	2.534282	0.993300	-1.257211
H	-0.559836	0.909029	-2.432544
H	2.425664	-0.939485	-0.487296
H	-0.585387	-1.037607	3.109468
H	1.273800	0.022022	2.958147
H	-3.100822	0.608424	0.730414
H	-2.899060	-1.344096	-0.181482
H	1.711137	-0.020789	-2.987774
H	1.585061	1.744128	-3.040292
H	3.557068	0.812270	-1.601740
H	2.477827	1.984705	-0.800693
H	-0.004164	-1.547289	0.316604
H	-0.583348	1.111098	2.989146
H	-2.801360	0.445439	-1.403448
H	2.667247	0.191533	0.662734

PdN -1002.96587315 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	0.002064	-0.003208	0.003475
P	-0.003830	0.022038	2.488020
N	2.155181	-0.005967	-0.224387
P	-2.353975	-0.241845	-0.243816
N	0.132662	0.831973	-1.762973
C	1.452583	0.815254	-2.398065
C	2.487420	0.989341	-1.305376
H	-0.611027	0.762341	-2.459699
H	2.432645	-0.948637	-0.511794
H	-1.040418	-0.659949	3.149396
H	1.148183	-0.503637	3.100313
H	-3.098502	0.667812	0.527943
H	-2.877584	-1.499708	0.097166
H	1.611667	-0.109585	-2.973505
H	1.492529	1.642786	-3.122504
H	3.508524	0.824711	-1.663496
H	2.420247	1.986873	-0.864491
H	-0.009637	-1.484461	0.399452
H	-0.087237	1.328038	3.010186
H	-2.804880	-0.022800	-1.556455
H	2.685204	0.198296	0.624379

PtN -995.433764537 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.001301	0.004069	0.008842
P	-0.001382	0.002964	2.453858
N	2.154055	0.007570	-0.211723
P	-2.356160	-0.107171	-0.193143
N	0.154451	0.880445	-1.713575
C	1.475349	0.943709	-2.356643
C	2.511525	1.041879	-1.253284
H	-0.606907	0.946632	-2.387775
H	2.431123	-0.925252	-0.531471
H	-1.005214	-0.738364	3.100357
H	1.176605	-0.486676	3.044946
H	-3.079623	0.609951	0.774720
H	-2.877002	-1.409623	-0.131914
H	1.638522	0.064699	-2.996762
H	1.510899	1.827664	-3.005660
H	3.528502	0.863539	-1.614207
H	2.468720	2.018956	-0.766211
H	-0.014456	-1.509991	0.411489
H	-0.137884	1.294271	2.997357
H	-2.821510	0.405349	-1.415486
H	2.680635	0.177962	0.646682

FeN-H2 -1001.44042910 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Fe	0.042702	-0.038902	-0.030421
P	0.026614	0.023603	2.208792
N	2.112058	-0.014160	-0.120485
P	-2.138369	-0.408577	-0.233219
N	0.221406	-0.258282	-2.008213
C	1.551617	-0.732774	-2.348820
C	2.536099	0.100930	-1.544485
H	-0.449191	-0.912073	-2.407882
H	2.373470	-0.932133	0.234291
H	-0.845428	-0.860335	2.893781
H	1.212341	-0.391491	2.878639
H	-3.147516	0.594459	-0.303176
H	-2.808240	-1.224368	0.714369
H	1.733885	-1.802620	-2.104459
H	1.780872	-0.615469	-3.423124
H	3.578777	-0.215394	-1.682663
H	2.444460	1.154007	-1.830180
H	0.106571	-1.545474	0.187837
H	-0.212067	1.138070	3.069684
H	-2.544664	-1.117801	-1.390701
H	2.590641	0.675758	0.455344
H	-0.009566	1.810411	-0.058246
H	-0.033255	1.596155	-0.804706

RuN-H2 -971.940895935 a.u.

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.008736	-0.060355	0.000824
P	-0.021252	0.026318	2.330888
N	2.220290	-0.042152	-0.157928
P	-2.229161	-0.421937	-0.225416
N	0.257798	-0.267999	-2.104293
C	1.593728	-0.772623	-2.388933
C	2.586990	0.068281	-1.600933
H	-0.412679	-0.918829	-2.511318
H	2.518214	-0.947010	0.200769
H	-0.773727	-0.935806	3.057672
H	1.197367	-0.202253	3.035362
H	-3.207064	0.609779	-0.163114
H	-2.911914	-1.328363	0.627151
H	1.756308	-1.836611	-2.110566
H	1.841317	-0.689412	-3.462048
H	3.626986	-0.240785	-1.771750
H	2.476319	1.119588	-1.885560
H	0.122024	-1.645600	0.151992
H	-0.416406	1.129807	3.145490
H	-2.669236	-0.981126	-1.454659
H	2.698570	0.667177	0.393519
H	-0.027241	1.938202	-0.001865
H	-0.112748	1.755249	-0.753327

OsN-H2 -969.116495637 a.u.

Coordinates (Angstroms)			
	X	Y	Z

Os	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.273605
N	2.144454	0.000000	-0.050090
P	-2.293483	0.238946	-0.179848
N	0.397556	0.256905	-2.160589
C	1.858771	0.066899	-2.428457
C	2.612172	0.670168	-1.252613
H	-0.158597	-0.339419	-2.769859
H	0.474557	-1.790198	0.015824
H	-0.321195	-1.138660	3.064283
H	1.233232	0.298093	2.916659
H	-2.958329	1.233549	0.590379
H	-3.264107	-0.778871	0.054787
H	2.044256	-1.011206	-2.464148
H	2.139373	0.515263	-3.389818
H	3.692871	0.516889	-1.413177
H	2.439174	1.769177	-1.268643
H	0.080955	1.633328	0.066020
H	-0.277396	-1.817062	-0.318612
H	-0.799785	0.923103	2.998690
H	-2.848344	0.645815	-1.431166
H	2.547638	0.475512	0.755061
H	0.140128	1.218057	-2.376506

IrN-H2 -982.581085519 a.u.

Coordinates (Angstroms)

	X	Y	Z
Ir	-0.001737	0.008978	-0.000503
P	0.002010	-0.001260	2.303830
N	2.058539	0.005433	-0.017186
P	-2.370046	-0.043924	-0.204077
N	0.355328	0.197124	-2.129342
C	1.813786	-0.065428	-2.405117
C	2.596976	0.557865	-1.264848
H	-0.225517	-0.402479	-2.714989
H	0.610710	-2.051105	-0.080960
H	-0.394271	-1.170070	2.985511
H	1.259738	0.226007	2.897047
H	-3.116946	0.857222	0.582820
H	-3.122920	-1.216062	0.037251
H	1.951814	-1.149846	-2.410032
H	2.088710	0.337388	-3.384492
H	3.658325	0.294164	-1.365157
H	2.528006	1.658212	-1.335788
H	-0.078734	1.559146	0.085226
H	-0.137940	-2.154712	-0.181172
H	-0.782613	0.959156	2.970885
H	-2.900975	0.287743	-1.470247
H	2.495045	0.485692	0.767029
H	0.132116	1.155809	-2.398520

PdN-H2 -1004.14500088 a.u.

Coordinates (Angstroms)

X	Y	Z

Pd	0.061951	-0.281272	-0.043953
P	-0.033026	0.056661	2.465733
N	2.210269	-0.278524	-0.143021
P	-2.289900	-0.512119	-0.256898
N	0.263399	-0.327780	-2.058552
C	1.635416	-0.671451	-2.467525
C	2.588031	0.078356	-1.560744
H	-0.386882	-0.957026	-2.536727
H	2.562254	-1.209994	0.092662
H	-0.220450	-1.119854	3.214657
H	1.134269	0.588448	3.047167
H	-2.948748	0.713771	-0.055886
H	-2.914032	-1.405543	0.629126
H	1.837610	-1.751429	-2.460614
H	1.745479	-0.333035	-3.509735
H	3.635874	-0.181575	-1.739752
H	2.464346	1.158137	-1.670998
H	0.028396	-1.795296	0.032707
H	-1.023880	0.906330	2.995256
H	-2.701782	-0.930694	-1.532815
H	2.648279	0.366961	0.517659
H	-0.021006	2.292635	0.129398
H	-0.066484	2.177581	-0.609968

TS (Fe) -1001.42970745 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Fe	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.211953
N	2.046759	0.000000	-0.083691
P	-2.210093	-0.216036	-0.179437
N	0.231306	0.478335	-2.006798
C	1.659617	0.373385	-2.409297
C	2.506522	0.784636	-1.209812
H	-0.355524	-0.046947	-2.650735
H	1.260903	-1.141547	-0.229270
H	0.071536	-1.132945	3.075750
H	1.057641	0.719931	2.823307
H	-3.067722	0.442441	0.739747
H	-2.908069	-1.456773	-0.167616
H	1.854414	-0.676449	-2.651210
H	1.878734	0.982307	-3.295894
H	3.568936	0.609540	-1.449837
H	2.382780	1.872823	-1.045725
H	-0.246634	1.522531	0.253985
H	0.414760	-1.639598	-0.279630
H	-1.062357	0.640059	2.898925
H	-2.845854	0.284034	-1.352114
H	2.561512	0.192165	0.768419
H	-0.070619	1.448980	-2.037943

TS (Ru) -971.922783058 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Ru	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.272209
N	2.188462	0.000000	-0.154202
P	-2.269317	-0.269115	-0.166372
N	0.306577	0.377079	-2.164579
C	1.743224	0.200605	-2.514433
C	2.598631	0.703592	-1.354063
H	-0.279214	-0.184151	-2.778461
H	1.476096	-1.191410	-0.203179
H	-0.084754	-1.170347	3.077661
H	1.140135	0.546320	2.921387
H	-3.171977	0.452232	0.662088
H	-2.924506	-1.525720	-0.025030
H	1.912664	-0.871712	-2.653660
H	1.995039	0.718307	-3.449017
H	3.658082	0.525413	-1.604594
H	2.463487	1.798764	-1.266050
H	-0.291073	1.607148	0.123352
H	0.653026	-1.759141	-0.209261
H	-0.970973	0.747171	2.988419
H	-2.904434	0.075608	-1.395430
H	2.717878	0.271379	0.667366
H	0.030683	1.348650	-2.283938

TS (Os) -969.097657553 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.265358
N	2.198102	0.000000	-0.193263
P	-2.252724	-0.293547	-0.149673
N	0.292886	0.333377	-2.167499
C	1.724538	0.147301	-2.549143
C	2.602495	0.670310	-1.415383
H	-0.303118	-0.246488	-2.754888
H	1.444863	-1.190397	-0.201118
H	-0.189940	-1.160182	3.070847
H	1.183277	0.441843	2.923142
H	-3.174655	0.488057	0.604709
H	-2.895818	-1.541375	0.098652
H	1.887858	-0.927844	-2.673455
H	1.948903	0.649422	-3.498014
H	3.655538	0.472337	-1.673178
H	2.477815	1.768222	-1.350500
H	-0.280225	1.637008	0.066771
H	0.598414	-1.742932	-0.192899
H	-0.906056	0.829297	2.979305
H	-2.882200	-0.066960	-1.412097
H	2.726029	0.302674	0.617863
H	0.015326	1.300297	-2.320109

TS (Co) -1022.87278246 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Co	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.241871
N	1.966924	0.000000	-0.029277
P	-2.276897	-0.293774	-0.162200
N	0.201041	0.398254	-1.968666
C	1.646521	0.329539	-2.362447
C	2.450138	0.787436	-1.156398
H	-0.348763	-0.212858	-2.571139
H	1.219624	-1.219778	-0.176908
H	0.288843	-1.185203	2.950237
H	0.934766	0.877108	2.823212
H	-2.875710	0.030860	-1.398702
H	-3.110443	0.455174	0.692350
H	1.874746	-0.714724	-2.591806
H	1.836002	0.935832	-3.253017
H	3.520625	0.611944	-1.327343
H	2.307201	1.869303	-1.000789
H	-0.236229	1.433630	0.227117
H	0.385839	-1.674968	-0.206469
H	-1.171392	0.408583	2.909269
H	-2.830129	-1.576866	0.028937
H	2.459547	0.209817	0.833629
H	-0.149777	1.343808	-2.114537

TS (Rh) -987.343167387 a.u.

Coordinates (Angstroms)

	X	Y	Z
Rh	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.312216
N	2.120166	0.000000	-0.093870
P	-2.341947	-0.304397	-0.170381
N	0.289710	0.301020	-2.131809
C	1.745082	0.151974	-2.463749
C	2.555567	0.699957	-1.298422
H	-0.264372	-0.323856	-2.715658
H	1.447780	-1.256425	-0.142559
H	-0.956128	0.794597	2.972437
H	-0.165998	-1.221982	2.993850
H	-3.194282	0.414145	0.691980
H	-2.878313	-1.598894	-0.010407
H	1.942301	-0.916011	-2.588837
H	1.978835	0.664436	-3.401958
H	3.624419	0.523273	-1.481049
H	2.405604	1.789304	-1.221604
H	-0.290662	1.537701	0.122443
H	0.632359	-1.780565	-0.142159
H	1.181469	0.469784	2.918774
H	-2.932702	0.039943	-1.404836
H	2.618057	0.301925	0.738559
H	-0.019307	1.249041	-2.341783

TS (Ir) -982.564527719 a.u.

Coordinates (Angstroms)

	X	Y	Z

Ir	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.300419
N	2.136514	0.000000	-0.114684
P	-2.311985	-0.305615	-0.167677
N	0.298322	0.265499	-2.135152
C	1.753564	0.104331	-2.484173
C	2.578627	0.666792	-1.336687
H	-0.261428	-0.361160	-2.712448
H	1.408203	-1.284393	-0.138373
H	-0.264431	-1.197143	2.995728
H	1.218954	0.375309	2.900244
H	-3.163287	0.457083	0.657444
H	-2.856853	-1.588700	0.047746
H	1.942400	-0.966800	-2.595492
H	1.969931	0.602033	-3.433724
H	3.641971	0.468933	-1.524464
H	2.443817	1.760103	-1.285276
H	-0.299851	1.565103	0.081673
H	0.587653	-1.778967	-0.132352
H	-0.887920	0.877482	2.950932
H	-2.893684	-0.014718	-1.420662
H	2.638646	0.325327	0.705654
H	-0.002967	1.212730	-2.361398

TS (Pd) -1004.11887129 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.378300
N	2.137411	0.000000	-0.044080
P	-2.418765	-0.336643	-0.212800
N	0.334598	0.257283	-2.130643
C	1.806248	0.112313	-2.423134
C	2.572992	0.700072	-1.251936
H	-0.200685	-0.404891	-2.695678
H	1.447068	-1.277737	-0.071053
H	1.160263	-0.574013	2.925987
H	-0.087438	1.270460	2.969972
H	-3.233872	0.346232	0.706684
H	-2.833111	-1.675765	-0.092005
H	2.016544	-0.954719	-2.528759
H	2.046383	0.614469	-3.364944
H	3.653877	0.532289	-1.372050
H	2.414897	1.786074	-1.181505
H	-0.332180	1.508373	0.104241
H	0.628103	-1.770040	-0.064841
H	-1.046385	-0.732549	2.964023
H	-2.952044	0.060495	-1.452339
H	2.592574	0.347221	0.800322
H	0.011062	1.191580	-2.389518

TS (Pt) -996.584642871 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Pt	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.369204
N	2.140703	0.000000	-0.075038
P	-2.408297	-0.366560	-0.192881
N	0.321675	0.198960	-2.140998
C	1.794658	0.045028	-2.455751
C	2.580755	0.657354	-1.310972
H	-0.218477	-0.472774	-2.690377
H	1.431613	-1.335571	-0.069325
H	1.252308	-0.332482	2.912571
H	-0.326322	1.238355	2.943634
H	-3.218551	0.337393	0.714260
H	-2.817758	-1.702716	-0.036224
H	1.998738	-1.025076	-2.541395
H	2.010654	0.525448	-3.413780
H	3.653982	0.465233	-1.442987
H	2.437687	1.747070	-1.275298
H	-0.326210	1.527726	0.059383
H	0.620367	-1.805055	-0.053916
H	-0.883040	-0.914745	2.966789
H	-2.949209	-0.002814	-1.438755
H	2.601844	0.384505	0.748456
H	0.000755	1.127240	-2.424933

FeHNH -1001.46058376 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Fe	0.046566	0.000794	-0.044293
P	0.049628	0.024899	2.163155
N	2.119783	-0.042873	-0.128876
P	-2.156780	-0.061230	-0.166086
N	0.240762	0.083295	-2.108937
C	1.619719	-0.283626	-2.488201
C	2.565344	0.355298	-1.479035
H	-0.425652	-0.531447	-2.567927
H	2.395125	-0.999937	0.076919
H	-0.356702	-1.065052	2.985796
H	1.301229	0.222030	2.820643
H	-3.019601	1.006927	0.213944
H	-2.912753	-1.082433	0.471126
H	1.694051	-1.374350	-2.427582
H	1.878427	0.024913	-3.510756
H	3.605637	0.069010	-1.687777
H	2.489105	1.445990	-1.537847
H	0.098296	1.613752	-0.000295
H	0.034516	-1.611495	-0.125908
H	-0.645097	1.021260	2.901410
H	-2.742946	-0.247294	-1.454280
H	2.531421	0.567512	0.571604
H	0.032708	1.041515	-2.378504

RuHNH -971.957330575 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Ru	-0.001199	-0.000031	0.001260
P	-0.000203	0.000017	2.260735
N	2.210863	0.000074	-0.150875
P	-2.257151	-0.039079	-0.118885
N	0.266599	0.042451	-2.199371
C	1.666786	-0.312820	-2.515629
C	2.593557	0.386026	-1.526136
H	-0.373897	-0.599197	-2.658424
H	2.525490	-0.942345	0.064899
H	-0.503293	-1.076977	3.044673
H	1.263458	0.070921	2.920694
H	-3.085882	1.015349	0.359563
H	-3.039360	-1.089773	0.438004
H	1.757270	-1.398402	-2.404952
H	1.944938	-0.045173	-3.544735
H	3.640498	0.141181	-1.754232
H	2.468124	1.471006	-1.603656
H	0.053099	1.718279	-0.037795
H	0.070386	-1.716171	-0.081712
H	-0.615345	1.027049	3.030668
H	-2.848518	-0.099703	-1.416583
H	2.624055	0.637797	0.523853
H	0.050563	0.986566	-2.508690

OsHNH -969.137338586 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	-0.001179	-0.000017	0.001123
P	-0.000068	-0.000133	2.253842
N	2.207957	0.000216	-0.162548
P	-2.250442	-0.039114	-0.117359
N	0.276678	0.043285	-2.196150
C	1.677666	-0.308761	-2.529171
C	2.606562	0.383786	-1.537901
H	-0.362545	-0.606442	-2.647396
H	2.538618	-0.935614	0.060708
H	-0.511136	-1.074518	3.041862
H	1.265136	0.063488	2.918759
H	-3.083404	1.011567	0.371219
H	-3.034320	-1.095414	0.434305
H	1.769506	-1.395092	-2.430089
H	1.941962	-0.027880	-3.557327
H	3.652028	0.125846	-1.753119
H	2.492374	1.469726	-1.615765
H	0.093997	1.721611	-0.079551
H	0.115998	-1.717923	-0.119796
H	-0.611459	1.031533	3.026131
H	-2.847703	-0.090331	-1.416419
H	2.613452	0.645836	0.510597
H	0.053639	0.980992	-2.521597

CoHNH -1022.92470858 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Co	-0.001340	0.000161	0.001165
P	-0.001091	-0.014253	2.234830
N	2.010434	0.012725	-0.076769
P	-2.230440	-0.133613	-0.051065
N	0.115755	0.129040	-2.004686
C	1.505246	-0.189684	-2.434872
C	2.444367	0.454332	-1.431007
H	-0.534517	-0.496896	-2.475441
H	2.344198	-0.932433	0.107045
H	-0.231176	-1.207390	2.951843
H	1.207610	0.390632	2.841211
H	-3.031031	0.991234	0.239455
H	-2.865814	-1.093222	0.762405
H	1.612359	-1.278205	-2.418158
H	1.704519	0.163346	-3.452192
H	3.487141	0.184893	-1.629292
H	2.355047	1.544049	-1.465041
H	-0.041360	1.543637	0.136881
H	-0.033247	-1.548122	-0.064499
H	-0.888931	0.844831	2.913061
H	-2.784564	-0.496219	-1.297680
H	2.425455	0.621959	0.625269
H	-0.126529	1.079971	-2.279499

RhHNH -987.396537312 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Rh	-0.000587	-0.000006	0.000535
P	-0.000695	-0.000110	2.291642
N	2.160317	0.000257	-0.133497
P	-2.289988	-0.027716	-0.083433
N	0.212318	0.028839	-2.153837
C	1.618687	-0.327019	-2.495920
C	2.549021	0.378100	-1.521905
H	-0.424952	-0.617075	-2.615093
H	2.497641	-0.935312	0.086862
H	-0.496305	-1.119212	2.990113
H	1.275749	0.104717	2.883716
H	-3.020091	1.075831	0.401350
H	-2.990394	-1.077726	0.542876
H	1.713087	-1.412542	-2.398191
H	1.858726	-0.050823	-3.528578
H	3.593184	0.117635	-1.727245
H	2.441034	1.463458	-1.606537
H	0.011767	1.667860	0.019893
H	0.002092	-1.667658	-0.032685
H	-0.666841	1.032429	2.981182
H	-2.833660	-0.121735	-1.382059
H	2.589720	0.643639	0.528128
H	-0.007420	0.965858	-2.487525

IrHNH -982.626108153 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Ir	-0.001575	-0.000017	0.001510
P	-0.000345	0.000495	2.284633
N	2.165046	0.000442	-0.141075
P	-2.282531	-0.015748	-0.096650
N	0.232769	0.015472	-2.157058
C	1.640952	-0.339406	-2.504844
C	2.569773	0.367376	-1.530834
H	-0.400413	-0.640365	-2.611042
H	2.513739	-0.928361	0.091499
H	-0.526368	-1.106549	2.981379
H	1.275485	0.072510	2.885614
H	-3.008655	1.082910	0.406736
H	-2.991066	-1.073216	0.509407
H	1.735708	-1.424823	-2.408557
H	1.874605	-0.059447	-3.537260
H	3.613085	0.095907	-1.722298
H	2.470071	1.452760	-1.622379
H	0.038619	1.679052	-0.018663
H	0.031947	-1.678598	-0.048950
H	-0.643288	1.048912	2.973844
H	-2.828351	-0.082841	-1.397297
H	2.587223	0.654868	0.515156
H	0.008755	0.945099	-2.509147

PdHNH -1004.18944006 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	-0.007606	0.000083	0.007377
P	-0.000379	0.195471	2.341164
N	2.143420	-0.245078	-0.146737
P	-2.336395	-0.235244	-0.070964
N	0.204051	0.285135	-2.133774
C	1.568556	-0.198561	-2.529402
C	2.569648	0.268893	-1.490803
H	-0.503369	-0.204126	-2.683024
H	2.364803	-1.238080	-0.057034
H	-0.144188	-1.021218	3.031182
H	1.197820	0.734874	2.836778
H	-3.051788	0.966529	0.074274
H	-2.900532	-1.092811	0.886827
H	1.529994	-1.290359	-2.580138
H	1.828446	0.183025	-3.522510
H	3.576311	-0.091257	-1.728151
H	2.600238	1.360557	-1.432340
H	0.101574	1.628510	0.206392
H	-0.175188	-1.629357	-0.135227
H	-0.989366	1.025818	2.892053
H	-2.787772	-0.761256	-1.292372
H	2.663569	0.240969	0.584498
H	0.103464	1.280162	-2.340937

PtHNH -996.664208774 a.u.

	Coordinates (Angstroms)		
	X	Y	Z

Pt	-0.002896	0.000089	0.002818
P	-0.002431	0.001064	2.347135
N	2.156699	-0.000533	-0.137219
P	-2.345557	0.032406	-0.078705
N	0.211232	-0.032941	-2.150431
C	1.629193	-0.396857	-2.496301
C	2.556364	0.337617	-1.547395
H	-0.422202	-0.700995	-2.591740
H	2.508448	-0.925800	0.116007
H	-0.655197	-1.084233	2.953329
H	1.299690	-0.056586	2.871775
H	-2.957799	1.135636	0.537326
H	-2.990796	-1.084964	0.475413
H	1.724186	-1.480970	-2.389738
H	1.838441	-0.130243	-3.536879
H	3.599493	0.053245	-1.716760
H	2.469038	1.421621	-1.661362
H	0.008426	1.662839	-0.010539
H	-0.013563	-1.662667	0.015519
H	-0.562015	1.135517	2.956864
H	-2.824226	0.078481	-1.398873
H	2.585735	0.670417	0.501563
H	-0.016168	0.890565	-2.523791

RH (Fe) -1194.64194125 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Fe	-0.134281	0.064562	-0.015076
P	-0.094615	-0.078910	2.186169
N	1.922403	-0.198648	-0.139518
P	-2.326197	0.310298	-0.106203
N	0.065061	0.384672	-2.056732
C	1.402740	-0.062186	-2.500365
C	2.405007	0.340584	-1.427910
H	-0.659811	-0.093072	-2.585002
H	2.154155	-1.190892	-0.078867
H	-0.488824	-1.207986	2.967689
H	1.170652	0.076707	2.824927
H	-3.037005	1.424435	0.426603
H	-3.221032	-0.672926	0.398805
H	1.377249	-1.152618	-2.583450
H	1.685817	0.355042	-3.476814
H	3.408826	-0.022846	-1.685164
H	2.439361	1.431832	-1.341100
H	0.111084	1.636658	0.224364
H	-0.381603	-1.506436	-0.294879
H	-0.772479	0.876383	2.989766
H	-2.928518	0.380953	-1.398843
H	2.391620	0.280056	0.624727
H	-0.044980	1.385422	-2.200149
H	0.074339	-3.555599	1.119996
C	0.968328	-4.167670	0.947760
C	1.459304	-3.864536	-0.449868
H	0.685737	-5.220668	1.054400
H	1.731585	-3.906302	1.683282

O	2.464990	-3.191971	-0.646100
C	0.629003	-4.395278	-1.597815
H	-0.337630	-3.877164	-1.582861
H	1.130751	-4.205766	-2.548603
H	0.435167	-5.467721	-1.483240

RH (Ru) -1165.13940442 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.000414	0.000325	-0.000089
P	-0.000224	0.000815	2.259017
N	2.212069	0.000804	-0.136386
P	-2.257713	0.071653	-0.134809
N	0.285862	0.149336	-2.192813
C	1.700913	-0.144921	-2.518946
C	2.598195	0.504991	-1.472733
H	-0.331755	-0.484109	-2.692190
H	2.577696	-0.944340	-0.009168
H	-0.319286	-1.125912	3.074939
H	1.233983	0.289824	2.913529
H	-3.032765	1.057105	0.539485
H	-3.105420	-1.020896	0.207275
H	1.829019	-1.230557	-2.480877
H	1.974822	0.203008	-3.524642
H	3.651155	0.294100	-1.703739
H	2.448741	1.589834	-1.474387
H	0.093675	1.712232	0.040487
H	0.003962	-1.715209	-0.165686
H	-0.779441	0.926508	3.007058
H	-2.840283	0.293606	-1.419004
H	2.612418	0.595354	0.584296
H	0.044549	1.101021	-2.456515
C	2.247471	-3.720305	-0.140869
O	3.114128	-2.902365	-0.429640
C	1.810201	-3.939251	1.289301
H	1.657372	-5.001077	1.509182
H	2.539623	-3.510577	1.979483
H	0.850339	-3.421424	1.412588
C	1.538730	-4.525904	-1.206904
H	1.582995	-5.597767	-0.982348
H	0.482409	-4.230785	-1.213849
H	1.980075	-4.331766	-2.186223

RH (Os) -1162.32018584 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	0.013660	-0.137568	0.050615
P	0.077594	-0.108383	2.301676
N	2.216670	-0.102251	-0.164884
P	-2.241334	-0.123137	-0.016184
N	0.242771	-0.032800	-2.149449
C	1.653381	-0.301937	-2.528413
C	2.570356	0.380469	-1.521281
H	-0.374488	-0.696891	-2.609360

H	2.611412	-1.035209	-0.026304
H	-0.248024	-1.220985	3.139969
H	1.338321	0.153559	2.924012
H	-3.026530	0.866130	0.647240
H	-3.051255	-1.225437	0.393266
H	1.805511	-1.384018	-2.483622
H	1.875655	0.042532	-3.546838
H	3.619240	0.170861	-1.766939
H	2.410482	1.463356	-1.540415
H	0.119209	1.580612	0.003690
H	0.083453	-1.855976	-0.113690
H	-0.658343	0.843014	3.067007
H	-2.873468	0.034927	-1.290073
H	2.622409	0.516979	0.532601
H	-0.032647	0.902052	-2.440743
H	1.007059	-3.421875	1.512596
C	1.952517	-3.964588	1.382723
C	2.348949	-3.805494	-0.066601
H	1.786499	-5.013297	1.649287
H	2.708368	-3.521516	2.034528
O	3.169264	-2.964578	-0.419391
C	1.661680	-4.703385	-1.070822
H	0.581167	-4.523053	-1.023776
H	2.026999	-4.497537	-2.078539
H	1.830577	-5.757914	-0.822596

RH (Co) -1216.11574857 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Co	-0.357414	0.430031	-0.003891
P	-0.326130	0.640366	2.212961
N	1.502416	-0.311592	-0.023606
P	-2.468074	1.158259	-0.104832
N	-0.230727	0.281334	-2.005846
C	0.945807	-0.563191	-2.356418
C	2.060785	-0.192990	-1.396416
H	-1.070424	-0.116520	-2.421161
H	1.509029	-1.302375	0.241680
H	-0.945939	-0.316054	3.045744
H	0.956529	0.655104	2.802343
H	-2.776552	2.526908	0.050010
H	-3.421141	0.609137	0.777541
H	0.659044	-1.607886	-2.210002
H	1.245079	-0.421040	-3.400413
H	2.925899	-0.850617	-1.526367
H	2.375085	0.844227	-1.548579
H	0.190469	1.883994	-0.032362
H	-0.976501	-0.983632	0.091059
H	-0.845045	1.816870	2.791729
H	-3.139414	0.915053	-1.323225
H	2.114503	0.180967	0.623182
H	-0.115430	1.218149	-2.389382
H	1.229732	-5.431331	1.869761
C	2.084115	-4.745400	1.810202
C	2.287696	-4.327243	0.372736
H	2.954531	-5.295902	2.183370

H	1.890968	-3.878069	2.443352
O	2.069998	-3.176707	0.000800
C	2.769798	-5.381782	-0.594345
H	2.167047	-6.292662	-0.508931
H	2.741413	-5.007524	-1.618597
H	3.799797	-5.662893	-0.341208

RH (Rh) -1180.58715125 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Rh	-0.380124	0.679207	-0.014845
P	-0.495650	0.710776	2.266940
N	1.577471	-0.217152	-0.011166
P	-2.438158	1.668634	-0.243865
N	-0.048510	0.568062	-2.151240
C	1.120995	-0.324236	-2.400466
C	2.183811	-0.028334	-1.356686
H	-0.861799	0.215362	-2.650726
H	1.517958	-1.223132	0.180372
H	-1.376953	-0.153794	2.947776
H	0.709107	0.381347	2.923965
H	-2.680686	2.910362	0.377944
H	-3.607400	0.981369	0.141869
H	0.776829	-1.356401	-2.295532
H	1.515013	-0.183781	-3.413175
H	3.042861	-0.694058	-1.490992
H	2.523271	1.009224	-1.432975
H	0.335391	2.193541	0.024757
H	-1.075641	-0.827913	-0.065179
H	-0.796165	1.920331	2.925811
H	-2.794703	2.001926	-1.568470
H	2.183154	0.200438	0.691690
H	0.141855	1.506852	-2.497061
H	0.980416	-5.332731	1.649009
C	1.900382	-4.761140	1.473708
C	1.937999	-4.302573	0.034616
H	2.734930	-5.437763	1.687856
H	1.928804	-3.908590	2.154032
O	1.844721	-3.114595	-0.264730
C	2.093983	-5.364536	-1.027274
H	1.364743	-6.169049	-0.880299
H	1.980045	-4.933689	-2.022896
H	3.087169	-5.822918	-0.942606

RH (Ir) -1175.81742308 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ir	-0.329824	0.353757	0.034769
P	-0.477114	0.538282	2.299542
N	1.718155	-0.332881	0.104653
P	-2.473555	1.071982	-0.291071
N	0.059616	0.114247	-2.087604
C	1.326229	-0.657860	-2.274456
C	2.333973	-0.179670	-1.243813

H	-0.701983	-0.368677	-2.559982
H	1.766097	-1.324305	0.366893
H	-1.327505	-0.321643	3.025739
H	0.730120	0.312551	2.997484
H	-2.852985	2.358045	0.146846
H	-3.553795	0.323325	0.221585
H	1.096660	-1.713126	-2.106456
H	1.711973	-0.534230	-3.291722
H	3.256322	-0.764505	-1.313882
H	2.568827	0.878842	-1.390411
H	0.258246	1.926996	-0.072321
H	-0.837571	-1.242456	0.076345
H	-0.846788	1.772594	2.873573
H	-2.881541	1.162419	-1.640738
H	2.266549	0.194721	0.780684
H	0.145732	1.035591	-2.513576
H	1.515426	-5.281178	2.133892
C	2.405754	-4.679691	1.911383
C	2.423343	-4.340890	0.439398
H	3.272972	-5.292441	2.180425
H	2.387163	-3.773567	2.518920
O	2.253830	-3.190501	0.041739
C	2.655928	-5.474268	-0.530310
H	1.983968	-6.312467	-0.314762
H	2.516296	-5.137195	-1.558295
H	3.678314	-5.853670	-0.409743

RH (Pd) -1197.39987837 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	-0.318088	0.574244	0.027604
P	-0.316340	0.380191	2.350103
N	1.647446	-0.251763	-0.167914
P	-2.597914	1.140490	-0.043161
N	0.010905	1.031705	-2.055820
C	1.226582	0.273033	-2.507803
C	2.260796	0.329401	-1.401934
H	-0.782962	0.792201	-2.649923
H	1.583806	-1.285699	-0.284053
H	-0.820253	-0.831082	2.855038
H	0.969845	0.467235	2.906944
H	-2.909520	2.468445	0.297950
H	-3.455728	0.380605	0.768740
H	0.925018	-0.761334	-2.690344
H	1.609948	0.705502	-3.437614
H	3.147238	-0.252939	-1.675263
H	2.569504	1.357077	-1.188866
H	0.258516	2.066684	0.429413
H	-0.936024	-0.904664	-0.316633
H	-1.035344	1.361763	3.050933
H	-3.160083	0.987761	-1.321577
H	2.246655	-0.052555	0.632800
H	0.162200	2.037267	-2.144772
H	1.778786	-5.450257	0.451126
C	2.486382	-4.698560	0.079067
C	1.906086	-4.026708	-1.135859

H	3.400038	-5.243666	-0.182761
H	2.699291	-3.979210	0.871575
O	1.593608	-2.828451	-1.128376
C	1.717161	-4.858885	-2.373294
H	1.215858	-5.803023	-2.134031
H	1.152863	-4.314720	-3.131412
H	2.700863	-5.128394	-2.779355

RH (Pt) -1189.87809956 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.351978	0.535944	-0.245088
P	-0.497407	-0.581493	1.801712
N	1.459142	-0.520268	-0.733446
P	-2.241092	1.851577	0.181945
N	-0.073059	1.255216	-2.268843
C	0.830920	0.285117	-2.974572
C	1.990402	-0.039020	-2.050516
H	-0.952096	1.332433	-2.781235
H	1.287313	-1.541769	-0.713841
H	-1.803092	-0.892211	2.214074
H	0.168972	-1.823155	1.697291
H	-2.171065	2.668705	1.321361
H	-3.457297	1.165540	0.332696
H	0.237888	-0.604768	-3.199277
H	1.186703	0.718990	-3.914291
H	2.637516	-0.803479	-2.491009
H	2.595937	0.852203	-1.861642
H	0.572494	1.773511	0.366236
H	-1.275515	-0.704419	-0.855906
H	0.055763	0.082690	2.908804
H	-2.508789	2.764980	-0.851788
H	2.162554	-0.347766	-0.015235
H	0.347397	2.185998	-2.249678
H	0.411404	-5.885274	1.314789
C	1.250419	-5.194360	1.470489
C	1.409854	-4.334629	0.249221
H	2.136536	-5.819865	1.622965
H	1.060622	-4.594110	2.361299
O	1.133911	-3.124666	0.279261
C	1.914320	-4.989194	-1.005898
H	1.379800	-5.926037	-1.196557
H	1.823024	-4.327568	-1.868675
H	2.969052	-5.261414	-0.868820

TSH (Fe) -1194.63815866 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Fe	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.210730
N	2.050102	0.000000	-0.087972
P	-2.208979	0.097775	-0.128598
N	0.198077	0.245567	-2.055644
C	1.613608	0.065015	-2.460855

C	2.492596	0.624987	-1.351579
H	-0.399210	-0.385230	-2.583443
H	2.344306	-0.988186	-0.083110
H	-0.193265	-1.136112	3.051283
H	1.184657	0.446124	2.863100
H	-2.952125	0.968967	0.712238
H	-3.091002	-1.013159	0.009642
H	1.800831	-1.008237	-2.553894
H	1.836520	0.545379	-3.422725
H	3.550001	0.422426	-1.570117
H	2.353859	1.707369	-1.262283
H	-0.009430	1.584080	0.149940
H	0.034111	-1.620520	-0.174362
H	-0.886486	0.852315	2.919742
H	-2.782028	0.562674	-1.349121
H	2.488089	0.472857	0.698341
H	-0.108707	1.196656	-2.243938
C	1.087424	-3.167818	-0.413388
O	2.246645	-2.769073	-0.646830
C	0.738198	-3.712443	0.964851
H	1.078906	-4.757819	1.007984
H	1.269079	-3.154200	1.738282
H	-0.335901	-3.687005	1.161385
C	0.217387	-3.663732	-1.562808
H	0.510870	-4.700759	-1.783941
H	-0.846177	-3.649051	-1.314505
H	0.398298	-3.070029	-2.461746

TSH (Ru) -1165.13486251 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.002977	0.004481	-0.004750
P	0.009725	-0.027656	2.257873
N	2.181933	0.008542	-0.150579
P	-2.271508	0.022810	-0.133099
N	0.276296	0.237760	-2.194975
C	1.699091	-0.018460	-2.536547
C	2.587996	0.580340	-1.453661
H	-0.329751	-0.375565	-2.733530
H	2.469806	-0.983070	-0.116257
H	-0.256470	-1.184539	3.046488
H	1.230425	0.309322	2.910744
H	-3.063074	0.942402	0.608927
H	-3.092136	-1.110125	0.135862
H	1.846411	-1.101728	-2.552645
H	1.964333	0.389317	-3.521139
H	3.640301	0.364456	-1.683564
H	2.457353	1.666625	-1.407147
H	0.003448	1.685960	0.088939
H	0.110154	-1.738554	-0.204626
H	-0.812597	0.852308	3.011726
H	-2.861965	0.317359	-1.397928
H	2.638198	0.510884	0.606721
H	0.019661	1.197027	-2.413258
C	1.244112	-3.203502	-0.347896
O	2.383225	-2.754993	-0.607418

C	0.935247	-3.703257	1.057396
H	1.335046	-4.724799	1.145091
H	1.438767	-3.081107	1.799780
H	-0.137134	-3.729188	1.263323
C	0.414577	-3.823564	-1.467340
H	0.781974	-4.848035	-1.629930
H	-0.648442	-3.869685	-1.220480
H	0.554982	-3.268923	-2.397730

TSH (Os) -1162.31346824 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.257621
N	2.179637	0.000000	-0.169086
P	-2.262026	-0.018025	-0.119884
N	0.282488	0.194658	-2.190927
C	1.708422	-0.042353	-2.552387
C	2.597042	0.565576	-1.474888
H	-0.316312	-0.442623	-2.710918
H	2.472636	-0.996051	-0.135777
H	-0.286268	-1.145878	3.059577
H	1.218971	0.332138	2.922494
H	-3.068606	0.895993	0.618079
H	-3.060592	-1.164583	0.170904
H	1.869360	-1.123483	-2.571320
H	1.949515	0.373738	-3.538433
H	3.648293	0.338361	-1.693884
H	2.472293	1.652485	-1.435765
H	0.010425	1.689688	0.019053
H	0.174665	-1.750795	-0.205605
H	-0.823905	0.897725	2.992752
H	-2.870979	0.248181	-1.385409
H	2.637761	0.503479	0.587244
H	0.004664	1.141874	-2.436734
C	1.198679	-3.119863	-0.327488
O	2.359115	-2.714834	-0.603952
C	0.911037	-3.634549	1.079616
H	1.309387	-4.657404	1.150344
H	1.427830	-3.020529	1.819945
H	-0.158114	-3.658266	1.304094
C	0.364237	-3.760890	-1.435938
H	0.733868	-4.785677	-1.586427
H	-0.698176	-3.805927	-1.183906
H	0.497821	-3.220188	-2.376141

TSH (Co) -1216.08647808 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Co	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.254433
N	1.932556	0.000000	-0.070436
P	-2.287108	-0.076759	-0.074070
N	0.135205	0.215577	-1.994283

C	1.563833	0.084340	-2.436169
C	2.426611	0.636147	-1.316691
H	-0.441507	-0.447455	-2.511289
H	2.155212	-1.133732	-0.135421
H	-0.452688	-1.133512	2.960490
H	1.255392	0.182925	2.867967
H	-3.014252	0.803700	0.752581
H	-2.974014	-1.277301	0.203687
H	1.771961	-0.979465	-2.565730
H	1.727283	0.602379	-3.385733
H	3.479544	0.382619	-1.485898
H	2.341467	1.725312	-1.243765
H	-0.065417	1.461137	0.146037
H	0.126936	-1.724796	-0.085216
H	-0.740366	1.008149	2.901264
H	-2.881765	0.242308	-1.313963
H	2.420239	0.403938	0.727300
H	-0.212246	1.145759	-2.224336
C	0.812146	-2.792167	-0.228703
O	2.079739	-2.461158	-0.388301
C	0.493161	-3.547701	1.070854
H	0.920082	-4.553804	0.994499
H	0.969800	-3.061321	1.926894
H	-0.583504	-3.645208	1.250340
C	0.137612	-3.421716	-1.458102
H	0.587385	-4.405448	-1.631178
H	-0.940527	-3.558195	-1.318606
H	0.317662	-2.825086	-2.357806

TSH (Rh) -1180.55938835 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.311317
N	2.091353	0.000000	-0.085377
P	-2.340844	-0.099019	-0.140016
N	0.268233	0.184908	-2.140689
C	1.716403	-0.022397	-2.477662
C	2.559364	0.584900	-1.370227
H	-0.303410	-0.468716	-2.674087
H	2.312628	-1.095827	-0.098972
H	-0.471599	-1.136084	2.998020
H	1.266296	0.148684	2.911357
H	-3.109142	0.849218	0.564998
H	-3.020082	-1.276992	0.233770
H	1.894808	-1.099192	-2.515749
H	1.951347	0.417196	-3.452076
H	3.615887	0.341160	-1.532291
H	2.457552	1.674418	-1.340572
H	-0.078819	1.578354	0.093543
H	0.226540	-1.825783	-0.101136
H	-0.714804	1.016424	2.973037
H	-2.884519	0.081460	-1.429559
H	2.575946	0.447580	0.690904
H	-0.024733	1.121944	-2.413681
C	0.999005	-2.887209	-0.181937

O	2.238495	-2.502284	-0.361109
C	0.702860	-3.569862	1.162781
H	1.169730	-4.561389	1.151432
H	1.157145	-3.010609	1.986055
H	-0.369790	-3.697338	1.345724
C	0.348225	-3.607601	-1.373768
H	0.838634	-4.580373	-1.493096
H	-0.723461	-3.777823	-1.225162
H	0.504609	-3.050543	-2.302527

TSH (Ir) -1175.78260926 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ir	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.299789
N	2.087696	0.000000	-0.097742
P	-2.322924	-0.140512	-0.150941
N	0.285395	0.171738	-2.143256
C	1.739072	-0.015003	-2.488566
C	2.572484	0.589639	-1.372419
H	-0.277124	-0.488927	-2.678488
H	2.332899	-1.186578	-0.118720
H	-0.493140	-1.121962	2.995528
H	1.269923	0.126338	2.899701
H	-3.113143	0.798643	0.543413
H	-2.982800	-1.327376	0.232044
H	1.927490	-1.089272	-2.542211
H	1.959366	0.439600	-3.458705
H	3.628753	0.339908	-1.525668
H	2.477114	1.681085	-1.351784
H	-0.117333	1.590994	0.057118
H	0.268296	-1.850701	-0.090063
H	-0.695604	1.033994	2.955543
H	-2.871672	0.016559	-1.442633
H	2.569123	0.444295	0.682761
H	-0.017665	1.103501	-2.424982
C	1.058866	-2.869632	-0.140122
O	2.303575	-2.447167	-0.304026
C	0.777916	-3.551981	1.204652
H	1.292588	-4.519300	1.209841
H	1.189915	-2.963253	2.029334
H	-0.289906	-3.729518	1.371790
C	0.473860	-3.631498	-1.335968
H	1.015876	-4.578250	-1.437678
H	-0.590102	-3.855133	-1.205952
H	0.618181	-3.073908	-2.266222

TSH (Pd) -1197.34458588 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.342463
N	2.081821	0.000000	-0.098768
P	-2.423453	-0.171368	-0.149050

N	0.238539	0.383141	-2.115064
C	1.704622	0.328243	-2.469925
C	2.490859	0.816190	-1.268287
H	-0.287731	-0.267997	-2.698355
H	2.354506	-1.454686	-0.381842
H	-0.423210	-1.197140	2.944586
H	1.265264	0.224511	2.910972
H	-3.056500	-1.109784	0.686120
H	-2.889360	-0.557009	-1.419583
H	1.945025	-0.712183	-2.692892
H	1.890834	0.937621	-3.359187
H	3.568154	0.668427	-1.430285
H	2.331343	1.887118	-1.095772
H	-0.049547	1.577968	0.212207
H	0.095639	-1.751246	-0.163124
H	-0.805419	0.978626	2.946905
H	-3.162801	0.999448	0.097772
H	2.522466	0.395759	0.733997
H	-0.133838	1.314716	-2.303743
C	1.149703	-3.002007	-0.310075
O	2.168697	-2.399395	-0.853802
C	1.238726	-3.378068	1.149494
H	1.837666	-4.298778	1.197721
H	1.770754	-2.626015	1.737360
H	0.261441	-3.599330	1.583439
C	0.360252	-3.896273	-1.224849
H	0.945208	-4.818501	-1.353146
H	-0.605182	-4.175697	-0.799271
H	0.235306	-3.452017	-2.213702

TSH (Pt) -1189.81587779 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.342066
N	2.087530	0.000000	-0.103822
P	-2.417267	-0.118513	-0.146484
N	0.255189	0.276698	-2.133939
C	1.725273	0.207617	-2.491241
C	2.515068	0.749104	-1.314217
H	-0.267231	-0.402834	-2.688088
H	2.383171	-1.510107	-0.336332
H	-0.546849	-1.135942	2.961445
H	1.286978	0.092862	2.897888
H	-3.044816	-1.248353	0.407034
H	-2.907641	-0.123655	-1.464937
H	1.963623	-0.841841	-2.668585
H	1.901095	0.778335	-3.407053
H	3.587676	0.577153	-1.471249
H	2.366738	1.829723	-1.200627
H	-0.056356	1.600110	0.127635
H	0.133730	-1.774716	-0.136679
H	-0.692707	1.070058	2.930177
H	-3.132928	0.944819	0.430834
H	2.529540	0.431690	0.708989
H	-0.115709	1.196810	-2.376158

C	1.114625	-2.989672	-0.230812
O	2.173020	-2.445150	-0.779548
C	1.192756	-3.352537	1.235070
H	1.772034	-4.284120	1.297811
H	1.738775	-2.603975	1.815022
H	0.209261	-3.546300	1.668840
C	0.324815	-3.898222	-1.134958
H	0.895743	-4.832433	-1.230610
H	-0.652006	-4.148873	-0.717081
H	0.220353	-3.478640	-2.137108

PH (Fe) -1194.65906146 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Fe	1.346508	-0.008377	0.078184
P	1.453301	-1.912426	-1.051649
N	0.229489	0.778841	-1.220401
P	2.035057	-0.890399	2.014293
N	1.428589	1.925046	0.778864
C	0.327013	2.721540	0.172779
C	0.191207	2.241579	-1.266281
H	1.451483	2.054495	1.788032
H	-1.364093	0.411012	-0.206278
H	0.515859	-2.985791	-0.989228
H	1.457681	-1.809768	-2.467334
H	3.059696	-1.873187	2.056968
H	1.174831	-1.546617	2.943162
H	-0.586261	2.488283	0.727645
H	0.519203	3.800633	0.236179
H	-0.749338	2.627895	-1.689799
H	1.012914	2.662097	-1.875401
H	2.826591	0.067251	-0.237397
H	-2.380209	-1.641369	0.192520
H	2.610938	-2.720779	-0.934689
H	2.630017	-0.024330	2.976320
H	0.112687	0.406687	-2.160492
H	2.329764	2.236899	0.419090
C	-2.970647	-0.707895	0.189303
O	-2.109766	0.396226	0.445707
C	-3.658502	-0.576930	-1.175268
H	-4.260780	0.338296	-1.208851
H	-2.918133	-0.526101	-1.981515
H	-4.315187	-1.433641	-1.370822
C	-3.977750	-0.772886	1.334912
H	-4.578546	0.143622	1.361050
H	-4.652705	-1.628221	1.218059
H	-3.458284	-0.866134	2.293861

PH (Ru) -1165.15489527 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.001029	-0.002068	0.000304
P	-0.001491	-0.000511	2.278268
N	2.059263	-0.002543	-0.062434

P	-2.275064	-0.398662	-0.222039
N	0.353007	0.279750	-2.162107
C	1.790164	0.003820	-2.458241
C	2.616610	0.549023	-1.301516
H	-0.251530	-0.257176	-2.780778
H	2.448918	-1.768398	-0.189653
H	-0.339896	-1.130430	3.074796
H	1.229751	0.281379	2.931626
H	-3.269667	0.387417	0.425478
H	-2.881625	-1.650069	0.091381
H	1.911376	-1.082394	-2.504702
H	2.091308	0.439162	-3.419945
H	3.666603	0.249177	-1.448424
H	2.592696	1.654096	-1.324929
H	-0.422358	1.513455	0.092648
H	0.512682	-2.682484	-0.082473
H	-0.791458	0.933849	2.996275
H	-2.859747	-0.298389	-1.519388
H	2.579991	0.364780	0.732511
H	0.145250	1.263254	-2.326921
C	1.354353	-3.407828	-0.071534
O	2.556010	-2.736975	-0.410893
C	1.443412	-4.007789	1.337547
H	2.263243	-4.733771	1.382438
H	1.647142	-3.225316	2.076136
H	0.511932	-4.515173	1.618473
C	1.076543	-4.477163	-1.129705
H	1.906027	-5.192897	-1.163603
H	0.153743	-5.026974	-0.909956
H	0.985116	-4.022629	-2.121752

PH (Os) -1162.33201859 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	-0.088422	0.479214	0.040459
P	-0.210677	0.272249	2.290483
N	1.858050	0.041451	-0.031253
P	-2.301249	-0.001143	-0.328097
N	0.373495	0.831353	-2.080781
C	1.680638	0.192350	-2.428715
C	2.618342	0.376605	-1.241585
H	-0.352921	0.519507	-2.723093
H	1.790451	-1.964825	-0.402047
H	-1.051569	-0.672031	2.947917
H	0.979723	-0.072555	2.998309
H	-3.426341	0.839566	-0.056075
H	-2.885307	-1.175701	0.226415
H	1.489519	-0.873964	-2.574808
H	2.096632	0.615601	-3.351134
H	3.488310	-0.282511	-1.370819
H	2.994178	1.414145	-1.213886
H	-0.712374	1.966848	0.167746
H	0.210763	-3.570404	-0.003027
H	-0.561284	1.384356	3.103324
H	-2.677635	-0.272162	-1.679505
H	2.464994	0.012041	0.784799

H	0.439474	1.843901	-2.183685
C	1.267492	-3.861002	-0.125427
O	1.958986	-2.831068	-0.832146
C	1.875308	-4.083747	1.264171
H	2.928044	-4.374960	1.174184
H	1.824560	-3.167844	1.863634
H	1.340126	-4.872401	1.807061
C	1.332109	-5.117599	-0.989210
H	2.375250	-5.418164	-1.140563
H	0.796634	-5.947412	-0.514783
H	0.885973	-4.930174	-1.970976

PH (Co) -1216.11868462 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Co	0.230924	-0.166370	-0.154209
P	-0.247317	-0.081951	2.049768
N	2.060760	0.232819	0.217652
P	-1.975139	-0.709422	-0.727256
N	0.761858	0.048392	-2.074032
C	2.253945	0.176362	-2.163348
C	2.691225	0.922459	-0.916646
H	0.445743	-0.738320	-2.639656
H	1.919687	-1.674805	0.092543
H	-0.364457	-1.275607	2.796187
H	0.679002	0.610473	2.854421
H	-2.940524	0.310407	-0.597226
H	-2.680142	-1.751075	-0.084853
H	2.664145	-0.835903	-2.165229
H	2.546537	0.678303	-3.090762
H	3.785920	0.895478	-0.824079
H	2.397302	1.981554	-0.993384
H	-0.142029	1.225844	-0.113410
H	0.599077	-3.306200	1.399790
H	-1.436513	0.558413	2.452023
H	-2.241502	-1.082612	-2.064199
H	2.225996	0.791707	1.052771
H	0.321390	0.886670	-2.451022
C	0.963669	-3.460744	0.373553
O	1.125344	-2.155046	-0.250949
C	2.312565	-4.172675	0.423803
H	2.702296	-4.334975	-0.586457
H	3.048407	-3.594352	0.993186
H	2.207188	-5.146837	0.911581
C	-0.080025	-4.231005	-0.423547
H	0.258407	-4.384532	-1.453531
H	-0.252520	-5.211783	0.029679
H	-1.039948	-3.705143	-0.446278

PH (Rh) -1180.57293682 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.111734	-0.164231	-0.024623
P	0.062442	-0.147071	2.293596

N	2.124467	0.046943	-0.008839
P	-2.245473	-0.625418	-0.264190
N	0.439869	0.070687	-2.147478
C	1.917302	-0.020935	-2.412702
C	2.624790	0.659286	-1.254897
H	-0.061921	-0.600774	-2.727625
H	2.614385	-1.824885	-0.198575
H	-0.249215	-1.344040	2.969583
H	1.274529	0.192790	2.926535
H	-3.171187	0.126779	0.488879
H	-2.760493	-1.916462	-0.013657
H	2.175712	-1.082081	-2.435356
H	2.159954	0.435940	-3.377347
H	3.707981	0.495686	-1.339020
H	2.458029	1.747101	-1.291174
H	-0.210709	1.324833	0.070945
H	0.505509	-2.411982	-0.072382
H	-0.821082	0.742501	2.934447
H	-2.802463	-0.419900	-1.545461
H	2.516545	0.555940	0.782685
H	0.096541	0.992937	-2.415824
C	1.274985	-3.242590	-0.107276
O	2.491122	-2.718519	-0.593287
C	1.423792	-3.794355	1.313503
H	2.134864	-4.626457	1.309431
H	1.817907	-3.031353	1.994085
H	0.467994	-4.159838	1.706599
C	0.768219	-4.288539	-1.095934
H	1.500134	-5.098621	-1.176309
H	-0.184241	-4.717476	-0.768358
H	0.639250	-3.856371	-2.093086

PH (Ir) -1175.80899439 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ir	-0.023803	0.348905	-0.430803
H	-0.072937	-0.060604	1.079024
H	2.923473	-0.115561	0.756441
H	3.087354	0.711650	-1.230966
P	2.215605	0.729832	-0.120504
H	2.547114	1.988148	0.424417
H	0.802936	-2.368229	-2.159808
H	-0.943386	-2.711559	-0.972223
P	0.236947	-1.934866	-0.939722
H	0.990769	-2.737684	-0.057439
N	-0.466448	2.346726	-0.121981
C	-1.830232	2.514038	0.404182
H	0.177975	2.850170	0.484174
N	-2.184325	0.273505	-0.507601
C	-2.751411	1.669314	-0.458929
H	-2.522000	-0.202541	-1.343569
H	-2.521109	-0.261675	0.291905
H	-1.925476	2.208352	1.458813
H	-2.138872	3.566115	0.341513
H	-2.760600	2.044159	-1.484748
H	-3.777982	1.643696	-0.081746

O	-0.259383	1.359892	-2.546807
H	-0.301814	2.207226	-2.032130
C	0.576755	1.490423	-3.733261
H	1.616370	1.626228	-3.401942
C	0.134586	2.716336	-4.526986
H	-0.902255	2.606639	-4.861324
H	0.213297	3.629901	-3.927745
H	0.768885	2.842912	-5.410055
C	0.461048	0.197100	-4.525990
H	-0.574630	0.029401	-4.839702
H	1.086014	0.247508	-5.422577
H	0.792045	-0.662786	-3.936268

PH (Pd) -1197.38110572 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	-0.721871	-0.243024	-0.022501
H	-2.179096	-0.653915	-0.148682
H	-1.490775	-2.777476	1.862093
H	0.531547	-1.994512	2.312834
P	-0.754610	-1.582683	1.923512
H	-1.258919	-0.933438	3.063053
H	1.033439	-2.960299	-1.168194
H	0.286674	-1.792368	-2.848659
P	-0.060589	-2.151484	-1.532121
H	-1.061703	-3.113615	-1.761526
N	-1.234600	1.408453	1.102996
C	-1.925448	2.386029	0.242289
H	-1.872133	1.164785	1.865496
N	-0.982674	1.159502	-1.630857
C	-1.112780	2.535091	-1.026767
H	-0.187252	1.125877	-2.270598
H	-1.815742	0.928484	-2.175384
H	-2.966738	2.118472	0.015015
H	-1.954102	3.335832	0.798253
H	-0.103397	2.884992	-0.803304
H	-1.575600	3.214393	-1.748840
O	1.346840	0.649651	0.289427
H	1.154291	1.297154	0.989696
C	2.770681	0.216589	0.361403
H	2.776252	-0.735558	0.906444
C	3.560392	1.260195	1.137914
H	3.554965	2.226307	0.622651
H	3.173662	1.391671	2.154858
H	4.601723	0.937126	1.229754
C	3.262371	0.014744	-1.061555
H	3.281195	0.961861	-1.609397
H	4.278985	-0.389163	-1.049090
H	2.638299	-0.698343	-1.611607

PH (Pt) -1189.82340767 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.013402	0.449148	-0.393832

H	-0.044150	-0.010382	1.075693
H	2.944467	0.104878	0.910341
H	3.090301	0.841412	-1.173596
P	2.289105	0.924839	-0.022315
H	2.512454	2.228885	0.450294
H	1.432316	-2.164902	-2.011976
H	-0.685709	-2.550033	-1.649805
P	0.418932	-1.895891	-1.073291
H	0.754417	-2.767162	-0.021754
N	-0.495485	2.402905	0.047290
C	-1.893055	2.466074	0.523587
H	0.101225	2.813642	0.767070
N	-2.132552	0.281450	-0.534071
C	-2.737779	1.666503	-0.447059
H	-2.412191	-0.165623	-1.409060
H	-2.488220	-0.303768	0.224476
H	-2.022791	2.095765	1.550284
H	-2.203499	3.519397	0.516397
H	-2.694684	2.096820	-1.449232
H	-3.782735	1.585303	-0.135695
O	-0.104394	1.408401	-2.477416
H	-0.160248	2.338031	-2.183063
C	0.564059	1.312538	-3.808189
H	1.634055	1.174849	-3.609489
C	0.337942	2.620701	-4.552190
H	-0.727042	2.789089	-4.741476
H	0.746603	3.477923	-4.005469
H	0.848262	2.582737	-5.519320
C	-0.004371	0.099702	-4.523404
H	-1.072749	0.226094	-4.723580
H	0.504857	-0.033238	-5.482489
H	0.143769	-0.823417	-3.952018

Results calculated using PBEPBE/BSI

TS(Ru) -971.312928532 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.173614	-0.001820	0.032270
P	-1.684311	1.650967	-0.088764
N	1.533803	1.346752	0.306684
P	-1.751096	-1.621801	0.024686
N	1.525157	-1.385670	-0.200119
C	2.800054	-0.694634	0.148737
C	2.703975	0.757823	-0.318059
H	1.428342	-2.256102	0.332589
H	0.870101	0.756329	1.396938
H	-2.493470	2.107779	1.007958
H	-1.225066	2.957884	-0.468976
H	-2.867096	-1.601553	-0.879177
H	-2.530993	-1.986694	1.176644
H	2.892889	-0.718261	1.247823
H	3.675458	-1.205792	-0.292726
H	3.642645	1.280045	-0.031636
H	2.645886	0.767487	-1.432927
H	-0.254096	-0.032937	-1.608059
H	0.182641	0.166395	1.851690
H	-2.757540	1.585849	-1.035733
H	-1.364183	-2.973827	-0.290288
H	1.375360	2.318458	0.032515
H	1.512372	-1.629164	-1.195383

TS (Os) -968.497699868 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	0.137381	-0.002095	0.013443
P	1.676689	-1.638186	-0.077716
N	-1.579733	-1.352604	0.290826
P	1.698775	1.633123	0.025668
N	-1.566503	1.367394	-0.197807
C	-2.848123	0.687535	0.168012

C	-2.767852	-0.763978	-0.303008
H	-1.459160	2.234989	0.339340
H	-0.878104	-0.750383	1.377229
H	2.554659	-1.999057	1.003616
H	1.225688	-2.979879	-0.335190
H	2.773678	1.692538	-0.929086
H	2.525982	1.932647	1.164407
H	-2.925806	0.712861	1.268292
H	-3.718590	1.212214	-0.264905
H	-3.697205	-1.285969	0.008446
H	-2.734935	-0.772088	-1.419032
H	0.179653	0.047273	-1.652174
H	-0.173234	-0.136520	1.818004
H	2.695913	-1.621451	-1.086630
H	1.276231	2.997637	-0.181197
H	-1.420854	-2.318249	-0.002676
H	-1.577312	1.623751	-1.190573

TS(Rh) -986.726939230 a.u.

Coordinates (Angstroms)

	X	Y	Z
Rh	-0.150329	-0.002752	0.020429
P	-1.652225	1.713310	-0.075910
N	1.503122	1.320446	0.296299
P	-1.798235	-1.648657	0.013106
N	1.499634	-1.401251	-0.164694
C	2.788258	-0.702699	0.159643
C	2.678283	0.732578	-0.338838
H	1.394774	-2.239481	0.418702
H	0.836877	0.731254	1.462965
H	-2.679295	1.648757	-1.054261
H	-2.424918	2.031797	1.074199
H	-2.898673	-1.534700	-0.880132
H	-2.509631	-1.935223	1.211642
H	2.900035	-0.711290	1.255776
H	3.643077	-1.235185	-0.289149
H	3.589748	1.294538	-0.055858
H	2.611661	0.738856	-1.448584
H	-0.256094	-0.019795	-1.557143
H	0.160211	0.172335	1.863871
H	-1.119618	2.998707	-0.369775

H	-1.394958	-2.972828	-0.322649
H	1.342852	2.290232	0.008451
H	1.507131	-1.717548	-1.141349

TS (Ir) -981.960166227 a.u.

Coordinates (Angstroms)

	X	Y	Z
Ir	-0.122707	-0.001347	0.007251
P	-1.638499	1.699963	-0.063790
N	1.540783	1.327887	0.277698
P	-1.747170	-1.650137	0.013733
N	1.537567	-1.384356	-0.158773
C	2.832535	-0.691663	0.178124
C	2.734949	0.741324	-0.327005
H	1.431947	-2.225457	0.421357
H	0.828023	0.712616	1.469361
H	-2.505278	1.925376	1.040786
H	-1.094052	3.006268	-0.210871
H	-2.818475	-1.578411	-0.919176
H	-2.493922	-1.902420	1.198746
H	2.930802	-0.699343	1.275686
H	3.682520	-1.237667	-0.261876
H	3.639508	1.300318	-0.021262
H	2.695605	0.742613	-1.438607
H	-0.212902	-0.043116	-1.593235
H	0.150281	0.144024	1.847093
H	-2.580917	1.701943	-1.125937
H	-1.318451	-2.980911	-0.261217
H	1.383818	2.290600	-0.032483
H	1.561579	-1.702798	-1.135054

TS(Pd) -1003.50029048 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pd	-0.140088	-0.008663	0.007668
P	-1.630399	1.826365	-0.060409
N	1.540686	1.313321	0.276954

P	-1.880335	-1.698438	0.008338
N	1.503184	-1.432217	-0.138660
C	2.795657	-0.730950	0.186575
C	2.698996	0.688803	-0.351485
H	1.373796	-2.247244	0.476905
H	0.830040	0.739758	1.479390
H	-1.176319	2.955491	0.667544
H	-1.904957	2.330126	-1.355372
H	-2.998314	-1.462678	-0.830731
H	-2.471729	-1.943217	1.274851
H	2.904456	-0.723475	1.282474
H	3.642433	-1.285018	-0.251598
H	3.598710	1.277489	-0.075133
H	2.640370	0.691623	-1.459516
H	-0.284180	-0.060971	-1.545398
H	0.145931	0.211143	1.852282
H	-2.914075	1.581135	0.488551
H	-1.464826	-2.990721	-0.404383
H	1.390501	2.278996	-0.045109
H	1.518205	-1.787677	-1.105034

TS(Pt) -995.978559041 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pt	-0.112001	-0.001823	-0.008071
P	-1.622355	1.804282	-0.043117
N	1.572388	1.316854	0.275924
P	-1.840444	-1.698340	0.022252
N	1.537889	-1.420099	-0.134177
C	2.837591	-0.724308	0.206562
C	2.753095	0.695257	-0.329661
H	1.406669	-2.239092	0.476273
H	0.828129	0.719973	1.527454
H	-1.081124	2.996190	0.501055
H	-2.062611	2.172068	-1.337431
H	-2.950828	-1.481919	-0.831563
H	-2.442452	-1.926920	1.286045
H	2.932960	-0.722097	1.303852
H	3.678820	-1.290257	-0.225110
H	3.645487	1.275359	-0.022670
H	2.721372	0.699094	-1.438438

H	-0.228007	-0.055500	-1.575847
H	0.151951	0.185392	1.873329
H	-2.818423	1.618005	0.693740
H	-1.413364	-2.994306	-0.364890
H	1.422812	2.270770	-0.076766
H	1.570605	-1.776648	-1.100140

RuN -970.160620309 a.u.

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.159530	-0.015215	0.103474
P	-1.617511	1.704503	-0.206188
N	1.595347	1.266997	0.370998
P	-1.708703	-1.630949	-0.008130
N	1.315349	-1.293387	-0.329850
C	2.682656	-0.870475	-0.046523
C	2.757810	0.629614	-0.316882
H	1.224061	-2.313814	-0.286698
H	1.755955	1.295618	1.385070
H	-2.643883	2.150027	0.705234
H	-1.066336	3.025982	-0.387790
H	-2.775860	-1.657449	-0.972094
H	-2.535345	-1.960637	1.116238
H	2.992853	-1.066049	1.008535
H	3.422317	-1.388129	-0.692624
H	3.720238	1.065286	0.013470
H	2.628113	0.810857	-1.396842
H	-0.560882	0.199370	1.628989
H	-2.473588	1.774087	-1.361840
H	-1.262599	-2.975237	-0.264511
H	1.469827	2.236163	0.059177

OsN -967.349056101 a.u.

Coordinates (Angstroms)

	X	Y	Z
Os	-0.124913	-0.022437	0.129201
P	-1.486457	1.741656	-0.317239

N	1.666750	1.197806	0.402758
P	-1.758982	-1.543953	-0.068787
N	1.299620	-1.288789	-0.381289
C	2.703854	-0.927460	-0.192118
C	2.804052	0.587115	-0.357121
H	1.172947	-2.297004	-0.507692
H	1.872750	1.193537	1.410064
H	-2.457215	2.378198	0.549132
H	-0.840518	2.983661	-0.673470
H	-2.857560	-1.404383	-0.988115
H	-2.561058	-1.954497	1.050449
H	3.083668	-1.219550	0.814259
H	3.361902	-1.415750	-0.938209
H	3.778904	0.982665	-0.016381
H	2.652014	0.850652	-1.416472
H	-0.619962	0.310517	1.643754
H	-2.363743	1.709673	-1.456749
H	-1.398438	-2.877837	-0.483498
H	1.539293	2.178778	0.129185

RhN -985.578006791 a.u.

Coordinates (Angstroms)

	X	Y	Z
Rh	-0.131193	-0.011333	0.089933
P	-1.663876	-1.699434	-0.009782
N	1.318821	-1.271301	-0.311806
P	-1.706851	1.701598	-0.188910
N	1.559452	1.301418	0.352830
C	2.737036	0.668216	-0.330327
C	2.683559	-0.819492	-0.022612
H	1.424456	2.263288	0.020199
H	-2.622238	-1.720675	-1.061532
H	-1.126261	-3.008605	-0.155495
H	-1.253789	3.040106	-0.004182
H	-2.878850	1.779402	0.615084
H	2.610230	0.831950	-1.412370
H	3.680430	1.135813	-0.000262
H	3.407917	-1.363070	-0.658508
H	2.975523	-1.009381	1.032476
H	-0.545576	0.185479	1.570921
H	-2.523737	-1.905744	1.101541

H	-2.318896	1.864474	-1.466098
H	1.230492	-2.285450	-0.182402
H	1.733427	1.366755	1.364493

IrN -980.814173221 a.u.

Coordinates (Angstroms)

	X	Y	Z
Ir	0.110813	-0.016299	-0.116794
P	1.547714	1.748455	0.308043
N	-1.634694	1.212852	-0.410016
P	1.724187	-1.610055	0.055293
N	-1.286701	-1.272109	0.375182
C	-2.693239	-0.898672	0.181130
C	-2.781075	0.610778	0.356346
H	-1.160590	-2.285565	0.454879
H	-1.844380	1.203677	-1.417848
H	2.644155	2.098023	-0.532574
H	0.937199	3.034735	0.390683
H	2.782216	-1.461664	0.995539
H	2.473391	-1.929004	-1.108892
H	-3.056359	-1.200005	-0.823306
H	-3.335051	-1.402511	0.925961
H	-3.742061	1.023068	0.006619
H	-2.633005	0.877367	1.414696
H	0.640962	0.325498	-1.574180
H	2.226506	1.746552	1.560316
H	1.265933	-2.908155	0.420500
H	-1.514350	2.199191	-0.150315

PdN -1002.35302461 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pd	-0.128247	-0.015997	0.136758
P	-1.626769	1.840073	-0.320791
N	1.633249	1.170340	0.584062
P	-1.750509	-1.730845	0.049285
N	1.259201	-1.233444	-0.516677
C	2.647796	-0.884702	-0.222183

C	2.756225	0.629192	-0.259418
H	1.132406	-2.250161	-0.616687
H	1.833366	1.032266	1.586875
H	-2.986006	1.694767	0.054224
H	-1.279395	3.083984	0.265503
H	-2.990838	-1.391777	-0.547324
H	-2.120098	-2.258105	1.311622
H	2.968499	-1.302211	0.755759
H	3.301073	-1.360059	-0.982346
H	3.725955	0.993521	0.120490
H	2.610110	1.002136	-1.285162
H	-0.809132	0.375746	1.485317
H	-1.697410	2.134495	-1.709465
H	-1.334343	-2.867718	-0.689030
H	1.533059	2.185376	0.449877

PtN -994.834225964 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pt	0.096565	-0.018644	-0.122662
P	1.601011	1.811306	0.342589
N	-1.658192	1.203911	-0.467844
P	1.752392	-1.674536	0.040482
N	-1.291553	-1.256173	0.438730
C	-2.697913	-0.885898	0.230227
C	-2.789807	0.625631	0.347906
H	-1.157795	-2.271544	0.519472
H	-1.874349	1.144113	-1.475432
H	2.926036	1.720553	-0.152875
H	1.182465	3.075540	-0.145548
H	2.792430	-1.426601	0.970901
H	2.427821	-1.943228	-1.175041
H	-3.056192	-1.251024	-0.753486
H	-3.317960	-1.382296	1.000051
H	-3.751886	1.022279	-0.016211
H	-2.637992	0.945543	1.390603
H	0.724149	0.388943	-1.520524
H	1.784140	2.037722	1.732543
H	1.242254	-2.934725	0.441661
H	-1.541704	2.204829	-0.259532

RuHNH -971.341136696 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.175089	-0.000005	0.000051
P	-1.722132	-1.606973	-0.034847
N	1.514162	-1.406968	-0.069382
P	-1.722106	1.606988	0.034794
N	1.514159	1.406958	0.069381
C	2.746338	0.688176	-0.330982
C	2.746368	-0.688175	0.330877
H	1.347023	2.206047	-0.548568
H	1.583183	-1.750745	-1.031943
H	-2.659251	-1.792606	-1.110642
H	-1.277468	-2.979265	-0.020433
H	-2.658742	1.793371	1.110887
H	-2.698553	1.780731	-1.006628
H	2.710470	0.573939	-1.428335
H	3.668036	1.240918	-0.064135
H	3.668048	-1.240912	0.063958
H	2.710589	-0.573935	1.428233
H	-0.067496	-0.064863	1.712931
H	-0.067620	0.064841	-1.712850
H	-2.698115	-1.781401	1.006900
H	-1.277422	2.979264	0.019277
H	1.347075	-2.206042	0.548597
H	1.583248	1.750714	1.031945

OsHNH -968.530598531 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	-0.139902	-0.000003	0.000019
P	-1.687771	1.614615	0.034278
N	1.553033	1.397664	0.069833
P	-1.687795	-1.614598	-0.034315
N	1.553034	-1.397672	-0.069841
C	2.797127	-0.689452	0.327878
C	2.797113	0.689450	-0.327937
H	1.382885	-2.191055	0.556412

H	1.630217	1.758872	1.026310
H	-2.628318	1.805765	1.109915
H	-1.237865	2.988025	0.020037
H	-2.628582	-1.805374	-1.109806
H	-2.663904	-1.792705	1.010316
H	2.769610	-0.582805	1.426007
H	3.708526	-1.250409	0.047523
H	3.708521	1.250409	-0.047616
H	2.769553	0.582805	-1.426066
H	0.018210	0.062081	-1.717338
H	0.018254	-0.062089	1.717369
H	-2.664105	1.792395	-1.010196
H	-1.237915	-2.988021	-0.020611
H	1.382862	2.191057	-0.556405
H	1.630186	-1.758892	-1.026317

RhHNH -986.773730189 a.u.

Coordinates (Angstroms)

	X	Y	Z
Rh	-0.153492	0.000001	0.000049
P	-1.731708	1.619513	0.038327
N	1.488377	1.400905	0.063711
P	-1.731827	-1.619440	-0.038382
N	1.488373	-1.400936	-0.063663
C	2.735532	-0.684032	0.333224
C	2.735482	0.684012	-0.333364
H	1.335917	-2.202825	0.557068
H	1.569101	1.759901	1.021731
H	-2.604237	1.738430	1.155171
H	-1.238004	2.954695	-0.007307
H	-2.605182	-1.737178	-1.154691
H	-2.685581	-1.697725	1.013378
H	2.717176	-0.579010	1.430733
H	3.636412	-1.256985	0.052233
H	3.636409	1.256960	-0.052509
H	2.716953	0.578987	-1.430870
H	-0.131296	0.079502	-1.671426
H	-0.131213	-0.080596	1.671447
H	-2.686293	1.696880	-1.012762
H	-1.238163	-2.954688	0.005563
H	1.335873	2.202835	-0.556960

H	1.568957	-1.759967	-1.021679

IrHNH -982.014704223 a.u.

Coordinates (Angstroms)

	X	Y	Z
Ir	0.126366	0.000004	-0.000004
P	1.697997	1.626867	-0.043312
N	-1.527202	1.394150	-0.051481
P	1.698132	-1.626808	0.043332
N	-1.527207	-1.394209	0.051401
C	-2.783855	-0.682374	-0.336659
C	-2.783809	0.682336	0.336739
H	-1.373179	-2.185425	-0.583525
H	-1.613534	1.774547	-1.001218
H	2.582545	1.732565	-1.152900
H	1.202495	2.963236	-0.022989
H	2.582611	-1.732424	1.152968
H	2.642164	-1.722546	-1.016942
H	-2.771499	-0.574017	-1.433755
H	-3.676872	-1.263294	-0.050114
H	-3.676859	1.263260	0.050301
H	-2.771306	0.573979	1.433832
H	0.064931	0.064780	1.681895
H	0.065054	-0.065488	-1.681882
H	2.642019	1.722755	1.016972
H	1.202755	-2.963218	0.022948
H	-1.373154	2.185432	0.583361
H	-1.613446	-1.774686	1.001111

PdHNH -1003.56383947 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pd	-0.144766	-0.000003	-0.000011
P	-1.756194	-1.674944	0.108801
N	1.501993	-1.360496	-0.388062
P	-1.756161	1.674964	-0.108780
N	1.501986	1.360490	0.388058
C	2.746857	0.738632	-0.174438

C	2.746851	-0.738642	0.174462
H	1.364185	2.294676	-0.018606
H	1.585510	-1.485251	-1.406029
H	-2.406611	-1.967618	-1.117741
H	-1.237819	-2.927601	0.520822
H	-2.406445	1.967760	1.117804
H	-2.823119	1.459119	-1.014531
H	2.733542	0.892411	-1.265957
H	3.640536	1.241926	0.234104
H	3.640538	-1.241937	-0.234062
H	2.733515	-0.892422	1.265981
H	-0.179027	-0.366132	1.611240
H	-0.179158	0.366006	-1.611277
H	-2.823051	-1.459138	1.014680
H	-1.237788	2.927569	-0.520963
H	1.364169	-2.294678	0.018603
H	1.585478	1.485239	1.406027

PtHNH -996.050904492 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pt	0.114117	-0.000003	0.000001
P	1.736990	-1.668656	0.056141
N	-1.534992	-1.400759	0.020981
P	1.736976	1.668666	-0.056143
N	-1.534992	1.400756	-0.020983
C	-2.796208	0.671062	0.354452
C	-2.796206	-0.671066	-0.354455
H	-1.385486	2.182023	0.631151
H	-1.619531	-1.799946	0.966140
H	2.613144	-1.643566	1.168922
H	1.172592	-2.967677	0.115360
H	2.613142	1.643577	-1.168915
H	2.600230	1.736934	1.065092
H	-2.794244	0.549878	1.449962
H	-3.676875	1.271855	0.071196
H	-3.676875	-1.271859	-0.071201
H	-2.794241	-0.549881	-1.449964
H	0.107066	-0.042701	-1.670654
H	0.107048	0.042757	1.670653
H	2.600255	-1.736891	-1.065087

H	1.172555	2.967676	-0.115387
H	-1.385484	-2.182025	-0.631153
H	-1.619532	1.799942	-0.966141

Results calculated using mPW1PW91/BSI

TS (Ru) -971.896039428 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.168363	-0.003321	0.034440
P	-1.674116	1.660169	-0.085655
N	1.515386	1.335144	0.289645
P	-1.748804	-1.626480	0.021348
N	1.516985	-1.377542	-0.200324
C	2.777843	-0.690644	0.150278
C	2.686497	0.752367	-0.314700
H	1.426015	-2.242713	0.321307
H	0.862056	0.745327	1.391602
H	-2.410376	2.160910	1.020519
H	-1.215409	2.921881	-0.543250
H	-2.877265	-1.554921	-0.835385
H	-2.475037	-2.026096	1.175526
H	2.867830	-0.711954	1.239988
H	3.647627	-1.198772	-0.282243
H	3.613083	1.270446	-0.020540
H	2.642442	0.762374	-1.419743
H	-0.273044	-0.022370	-1.593772
H	0.199020	0.161508	1.844782
H	-2.777130	1.556814	-0.967781
H	-1.370831	-2.944044	-0.360504
H	1.374158	2.301500	0.027035
H	1.505978	-1.612636	-1.187003

TS (Os) -969.077660104 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	0.134765	-0.000774	0.016397
P	1.666545	-1.640910	-0.077223
N	-1.562826	-1.341368	0.277663
P	1.693890	1.631555	0.020794
N	-1.558948	1.358055	-0.197802
C	-2.826727	0.682134	0.165197

C	-2.748268	-0.760146	-0.302731
H	-1.456417	2.218339	0.331254
H	-0.870489	-0.738816	1.369392
H	2.470974	-2.054451	1.019630
H	1.218039	-2.943285	-0.427161
H	2.786848	1.632303	-0.887814
H	2.466266	1.970071	1.166009
H	-2.905867	0.705284	1.255757
H	-3.690742	1.202541	-0.261872
H	-3.666206	-1.279120	0.011989
H	-2.722901	-0.769940	-1.408222
H	0.192382	0.033939	-1.640327
H	-0.188552	-0.130666	1.806915
H	2.721806	-1.570791	-1.021171
H	1.282509	2.967215	-0.261388
H	-1.415783	-2.300789	-0.005339
H	-1.568113	1.608574	-1.181248

TS (Rh) -987.315756825 a.u.

Coordinates (Angstroms)

	X	Y	Z
Rh	-0.141377	-0.002566	0.019005
P	-1.640783	1.717407	-0.072236
N	1.476817	1.304526	0.278471
P	-1.796479	-1.649035	0.014331
N	1.481413	-1.390370	-0.171927
C	2.758312	-0.703490	0.164732
C	2.660368	0.725174	-0.326377
H	1.376416	-2.225891	0.397045
H	0.841259	0.729021	1.449335
H	-2.706875	1.612952	-0.981693
H	-2.333999	2.076316	1.097749
H	-2.903661	-1.501870	-0.840898
H	-2.462637	-1.953758	1.216362
H	2.860229	-0.715705	1.252262
H	3.608383	-1.233150	-0.272901
H	3.558036	1.279084	-0.024488
H	2.616455	0.735734	-1.426916
H	-0.258076	0.000228	-1.538937
H	0.180699	0.165869	1.855135
H	-1.110538	2.964897	-0.446629

H	-1.395114	-2.945486	-0.363180
H	1.331853	2.269375	0.006009
H	1.498782	-1.696934	-1.140865

TS (Ir) -982.544290192 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ir	-0.117556	-0.001561	0.008354
P	-1.633182	1.698056	-0.061915
N	1.516704	1.315576	0.262150
P	-1.739518	-1.649607	0.012884
N	1.522091	-1.371444	-0.163974
C	2.804434	-0.687730	0.178758
C	2.714169	0.738515	-0.319205
H	1.420040	-2.209234	0.403092
H	0.831972	0.708994	1.452580
H	-2.399631	1.992265	1.080577
H	-1.097230	2.968912	-0.340022
H	-2.829338	-1.529087	-0.868980
H	-2.427961	-1.939182	1.206359
H	2.898267	-0.697730	1.267172
H	3.649239	-1.228885	-0.253469
H	3.606189	1.291068	-0.001704
H	2.689909	0.743535	-1.420860
H	-0.219160	-0.027838	-1.579446
H	0.170337	0.136722	1.832580
H	-2.641590	1.625414	-1.037932
H	-1.316169	-2.949132	-0.330832
H	1.373117	2.274549	-0.029133
H	1.551116	-1.680559	-1.132357

TS (Pd) -1004.09025385 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	-0.130983	-0.008075	0.007196
P	-1.604749	1.815119	-0.063095
N	1.502347	1.291611	0.276419
P	-1.872010	-1.680306	0.012907

N	1.471450	-1.419034	-0.155166
C	2.757358	-0.735181	0.184034
C	2.670633	0.680674	-0.335635
H	1.341409	-2.234398	0.442693
H	0.831862	0.731545	1.466576
H	-1.162277	2.897120	0.713768
H	-1.818503	2.349754	-1.341603
H	-2.979737	-1.434409	-0.812902
H	-2.444253	-1.919642	1.273181
H	2.859056	-0.740381	1.271155
H	3.596309	-1.284607	-0.250032
H	3.555331	1.259136	-0.035961
H	2.625458	0.694913	-1.433377
H	-0.271313	-0.023305	-1.525201
H	0.152480	0.188963	1.840397
H	-2.892868	1.551948	0.426342
H	-1.453583	-2.954380	-0.404084
H	1.355180	2.249362	-0.033789
H	1.497552	-1.763337	-1.114524

TS (Pt) -996.561763703 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pt	-0.104849	-0.002001	-0.008253
P	-1.614742	1.789381	-0.041317
N	1.532848	1.302090	0.262117
P	-1.825655	-1.687965	0.023889
N	1.511867	-1.402450	-0.141755
C	2.802012	-0.718723	0.208578
C	2.724917	0.694773	-0.317185
H	1.383950	-2.219682	0.454516
H	0.834729	0.724394	1.504920
H	-1.076501	2.959275	0.515807
H	-2.034147	2.158246	-1.326761
H	-2.932810	-1.453449	-0.805322
H	-2.398000	-1.925648	1.283714
H	2.890727	-0.722446	1.296965
H	3.637389	-1.279523	-0.216009
H	3.601478	1.268079	0.007650
H	2.708939	0.703018	-1.415817
H	-0.220092	-0.034253	-1.559972

H	0.168177	0.177417	1.856486
H	-2.802477	1.586810	0.676852
H	-1.396430	-2.960421	-0.385521
H	1.389655	2.250485	-0.073896
H	1.555024	-1.751234	-1.099330

RuN -970.734859059 a.u.

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.154886	-0.009459	0.083333
P	-1.645649	1.693930	-0.184578
N	1.580760	1.275821	0.353035
P	-1.681303	-1.656348	-0.004622
N	1.326488	-1.283878	-0.306154
C	2.675155	-0.845455	-0.019792
C	2.738782	0.641078	-0.312932
H	1.248667	-2.292671	-0.237370
H	1.724103	1.299168	1.359060
H	-2.734349	1.979515	0.685951
H	-1.146509	3.028873	-0.188462
H	-2.701339	-1.744333	-0.990410
H	-2.523916	-1.925223	1.101735
H	2.974709	-1.015701	1.032431
H	3.422176	-1.360439	-0.642655
H	3.688266	1.086069	0.010394
H	2.617292	0.799584	-1.387763
H	-0.538702	0.183898	1.601222
H	-2.406953	1.843690	-1.377669
H	-1.203929	-2.983764	-0.173833
H	1.465378	2.236471	0.046895

OsN -967.920152966 a.u.

Coordinates (Angstroms)

	X	Y	Z
Os	-0.123201	-0.020505	0.126531
P	-1.481952	1.737895	-0.317201
N	1.661914	1.183626	0.409754
P	-1.752680	-1.544970	-0.065288

N	1.295186	-1.282307	-0.374186
C	2.688524	-0.921512	-0.197806
C	2.783456	0.584972	-0.352553
H	1.173695	-2.278001	-0.513993
H	1.860743	1.157810	1.407235
H	-2.452138	2.332292	0.546970
H	-0.845997	2.973877	-0.641596
H	-2.844899	-1.402742	-0.965110
H	-2.528014	-1.939773	1.055990
H	3.075293	-1.216337	0.793818
H	3.336381	-1.398288	-0.945858
H	3.751656	0.977065	-0.019841
H	2.628879	0.849938	-1.401240
H	-0.617568	0.308698	1.631384
H	-2.333915	1.711052	-1.455546
H	-1.395247	-2.861365	-0.477365
H	1.542303	2.160285	0.159300

RhN -986.159852203 a.u.

Coordinates (Angstroms)

	X	Y	Z
Rh	0.120642	0.008630	0.060575
P	1.622148	1.731708	-0.021338
N	-1.339322	1.262041	-0.253100
P	1.758533	-1.681456	-0.134170
N	-1.525108	-1.332333	0.283710
C	-2.712872	-0.686639	-0.339310
C	-2.675887	0.772325	0.050592
H	-1.388576	-2.265116	-0.096071
H	2.446182	1.853318	-1.156151
H	1.060400	3.020628	0.017993
H	1.367328	-2.994523	0.196593
H	2.939682	-1.616771	0.629310
H	-2.604506	-0.783157	-1.421931
H	-3.635352	-1.183496	-0.025750
H	-3.423940	1.330306	-0.525425
H	-2.937678	0.888307	1.114192
H	0.454902	-0.108639	1.542405
H	2.583315	1.834891	0.998968
H	2.327924	-1.937017	-1.398712
H	-1.261413	2.249634	-0.032854

H	-1.683827	-1.452562	1.282194

IrN -981.390006426 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ir	0.106499	-0.013398	-0.110774
P	1.558680	1.739402	0.296271
N	-1.617807	1.210131	-0.399572
P	1.706815	-1.622182	0.053118
N	-1.283461	-1.262748	0.356552
C	-2.677551	-0.885374	0.169070
C	-2.757044	0.614026	0.354884
H	-1.165544	-2.265970	0.435965
H	-1.823843	1.201505	-1.397606
H	2.702660	1.973044	-0.492047
H	0.994158	3.031044	0.246738
H	2.756429	-1.480946	0.980765
H	2.435549	-1.927925	-1.109231
H	-3.041063	-1.172337	-0.828585
H	-3.316736	-1.385645	0.903990
H	-3.707685	1.030722	0.012267
H	-2.611073	0.866735	1.407074
H	0.630077	0.318864	-1.554746
H	2.145934	1.794685	1.576020
H	1.237887	-2.901361	0.409772
H	-1.503159	2.187329	-0.144224

PdN -1002.93644313 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	0.111563	-0.015988	-0.113440
P	1.718270	1.778044	0.254334
N	-1.573273	1.248170	-0.470768
P	1.682036	-1.759996	-0.022214
N	-1.295727	-1.231897	0.418575
C	-2.659373	-0.817055	0.123278
C	-2.719744	0.678850	0.300448
H	-1.199641	-2.244543	0.373304

H	-1.773485	1.218286	-1.471946
H	3.044813	1.562558	-0.150365
H	1.405044	3.003919	-0.354420
H	2.518783	-1.704838	1.103895
H	2.564166	-1.839878	-1.109544
H	-2.965833	-1.124861	-0.886836
H	-3.334247	-1.329987	0.822204
H	-3.661107	1.107976	-0.052981
H	-2.578318	0.946418	1.349420
H	0.704450	0.285210	-1.487572
H	1.837713	2.103343	1.617644
H	1.101889	-3.035387	0.047031
H	-1.443032	2.231848	-0.240381

PtN -995.409946380 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pt	0.091078	-0.015596	-0.115582
P	1.618890	1.789124	0.317136
N	-1.626536	1.215293	-0.430376
P	1.722743	-1.685041	0.045479
N	-1.285261	-1.246553	0.402399
C	-2.680474	-0.867849	0.196072
C	-2.760716	0.630994	0.355408
H	-1.160134	-2.253250	0.461070
H	-1.843435	1.190135	-1.428779
H	2.933026	1.648642	-0.154052
H	1.230747	3.032096	-0.207140
H	2.722934	-1.462891	1.003995
H	2.421131	-1.917868	-1.147809
H	-3.030731	-1.195676	-0.791994
H	-3.302540	-1.373624	0.942679
H	-3.708206	1.043187	0.000479
H	-2.614330	0.915296	1.399207
H	0.693612	0.367237	-1.504952
H	1.779026	2.036580	1.691365
H	1.189775	-2.934554	0.395067
H	-1.509753	2.199861	-0.196007

RuHNH -971.931252521 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.171054	-0.000003	0.000048
P	-1.716665	-1.614446	-0.036062
N	1.508262	-1.398452	-0.065947
P	-1.716653	1.614453	0.036012
N	1.508261	1.398448	0.065946
C	2.727746	0.683452	-0.329858
C	2.727774	-0.683448	0.329759
H	1.344427	2.188007	-0.547658
H	1.576404	-1.739804	-1.018276
H	-2.635376	-1.791241	-1.105334
H	-1.266767	-2.966170	-0.020249
H	-2.634916	1.791926	1.105560
H	-2.677685	1.778895	-0.996790
H	2.695096	0.567302	-1.417243
H	3.641821	1.231338	-0.066976
H	3.641832	-1.231330	0.066809
H	2.695209	-0.567294	1.417147
H	-0.089753	-0.069276	1.703852
H	-0.089874	0.069250	-1.703778
H	-2.677262	-1.779527	0.997045
H	-1.266756	2.966166	0.019180
H	1.344475	-2.187999	0.547684
H	1.576468	1.739782	1.018277

OsHNH -969.117560349 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Os	-0.137963	-0.000002	0.000016
P	-1.681087	1.615254	0.035885
N	1.547006	1.388254	0.065662
P	-1.681104	-1.615242	-0.035918
N	1.547007	-1.388259	-0.065670
C	2.778425	-0.684589	0.326955
C	2.778413	0.684588	-0.327006
H	1.378840	-2.171603	0.556292
H	1.621574	1.746803	1.011923
H	-2.606525	1.793162	1.103018

H	-1.231110	2.970538	0.025180
H	-2.606731	-1.792848	-1.102935
H	-2.640855	-1.786031	1.000903
H	2.754207	-0.575447	1.415041
H	3.682122	-1.241066	0.050878
H	3.682118	1.241067	-0.050958
H	2.754159	0.575447	-1.415091
H	0.001459	0.065951	-1.708886
H	0.001502	-0.065957	1.708912
H	-2.641017	1.785773	-1.000812
H	-1.231145	-2.970535	-0.025648
H	1.378821	2.171605	-0.556287
H	1.621547	-1.746818	-1.011930

RhHNH -987.371022626 a.u.

Coordinates (Angstroms)

	X	Y	Z
Rh	0.146324	0.000000	0.000010
P	1.725979	-1.621729	0.043673
N	-1.476037	-1.390445	0.050118
P	1.725972	1.621734	-0.043683
N	-1.476039	1.390443	-0.050125
C	-2.713020	0.677554	0.336515
C	-2.713016	-0.677558	-0.336530
H	-1.327065	2.177819	0.573101
H	-1.559144	-1.758366	0.993550
H	2.593315	-1.715656	1.147142
H	1.226653	-2.938660	0.020862
H	2.593520	1.715418	-1.147007
H	2.656982	1.704055	1.007498
H	-2.697972	0.562992	1.423434
H	-3.605814	1.247613	0.062148
H	-3.605810	-1.247619	-0.062170
H	-2.697960	-0.562995	-1.423450
H	0.141300	-0.069698	-1.656849
H	0.141257	0.069644	1.656862
H	2.657189	-1.703793	-1.007349
H	1.226628	2.938666	-0.021279
H	-1.327052	-2.177816	-0.573112
H	-1.559137	1.758358	-0.993560

IrHNH -982.607438749 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Ir	0.121845	-0.000002	-0.000006
P	1.691566	-1.628056	0.043637
N	-1.513880	-1.382786	0.049480
P	1.691535	1.628071	-0.043620
N	-1.513882	1.382773	-0.049485
C	-2.759847	0.678449	0.334560
C	-2.759854	-0.678461	-0.334534
H	-1.363394	2.165727	0.579956
H	-1.601084	-1.762109	0.988481
H	2.561872	-1.723471	1.145498
H	1.194012	-2.947100	0.023761
H	2.561892	1.723491	-1.145441
H	2.621555	1.714651	1.009052
H	-2.750412	0.569048	1.421913
H	-3.644943	1.254399	0.050530
H	-3.644945	-1.254410	-0.050484
H	-2.750447	-0.569060	-1.421887
H	0.074414	-0.065866	-1.669386
H	0.074389	0.065931	1.669371
H	2.621636	-1.714579	-1.008996
H	1.193944	2.947103	-0.023800
H	-1.363401	-2.165732	-0.579972
H	-1.601108	1.762090	-0.988487

PdHNH -1004.16404633 a.u.

	Coordinates (Angstroms)		
	X	Y	Z
Pd	-0.139083	-0.000004	-0.000002
P	-1.742300	1.661218	-0.103465
N	1.480955	1.351321	0.373196
P	-1.742333	-1.661199	0.103473
N	1.480955	-1.351324	-0.373217
C	2.719107	-0.733758	0.176994
C	2.719119	0.733739	-0.176978
H	1.350189	-2.273398	0.037638

H	1.568763	1.488774	1.378920
H	-2.354726	1.959063	1.124386
H	-1.224847	2.889990	-0.538119
H	-2.354923	-1.958883	-1.124334
H	-2.813479	-1.427954	0.977173
H	2.709774	-0.878068	1.260174
H	3.603760	-1.234404	-0.227080
H	3.603763	1.234380	0.227121
H	2.709816	0.878048	-1.260158
H	-0.187124	0.354998	-1.595758
H	-0.186958	-0.354968	1.595748
H	-2.813568	1.427900	-0.976995
H	-1.224860	-2.890038	0.537915
H	1.350206	2.273388	-0.037681
H	1.568787	-1.488761	-1.378941

PtHNH -996.644410431 a.u.

Coordinates (Angstroms)

	X	Y	Z
Pt	-0.109002	-0.000004	-0.000008
P	-1.725921	-1.661492	-0.056300
N	1.513450	-1.386972	-0.019141
P	-1.725856	1.661524	0.056318
N	1.513454	1.386944	0.019153
C	2.767303	0.667870	-0.351559
C	2.767299	-0.667899	0.351575
H	1.369072	2.159813	-0.628209
H	1.602119	-1.788732	-0.951758
H	-2.604620	-1.613333	-1.147742
H	-1.160202	-2.942669	-0.141464
H	-2.604590	1.613348	1.147731
H	-2.561381	1.737217	-1.067183
H	2.768648	0.546322	-1.437437
H	3.639151	1.263643	-0.069285
H	3.639146	-1.263675	0.069305
H	2.768641	-0.546351	1.437453
H	-0.111380	-0.040654	1.655214
H	-0.111353	0.040789	-1.655224
H	-2.561478	-1.737075	1.067185
H	-1.160086	2.942674	0.141575
H	1.369053	-2.159833	0.628226

H 1.602121 1.788695 0.951775
