Correspondence and proofs to Professor Jennifer. C. Green
Email: jennifer.green@chem.ox.ac.uk

A DFT Based Investigation into the Electronic Structure and Properties of Hydride Rich Rhodium Clusters

S. K. Brayshaw[1], Jennifer C. Green*[2], Nilay Hazari[2] and Andrew S. Weller*[1]

[1]*Department of Chemistry, University of Bath, Bath, BA2 7AU U.K.*

[2]*Inorganic Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QR U.K.*

Comparison between S=0 and S=1 $[Rh_6(PH_3)H_{12}]$ (I)

Geometry optimizations were performed on $[Rh_6(PH_3)H_{12}]$ (**I**) with no unpaired electrons and with 2 unpaired electrons. The gas phase SCF energies indicated that the complex with 2 unpaired electrons was approximately 37 $kJmol^{-1}$ more stable than the complex with no unpaired electrons. In addition there was better agreement between complex with 2 unpaired electrons and the experimental structure than the complex with no unpaired electrons. This is clearly shown in Table S1.

Table SI: Selected experimental and calculated geometrical data for $[Rh_6(P^iPr_3)_6H_{12}]$ (**1a**) and $[Rh_6(PH_3)_6H_{12}]$ (**I**) with 2 unpaired electrons and no unpaired electrons.

	$[Rh_6(P^iPr_3)_6H_{12}]$ (1a)	**$[Rh_6(PH_3)_6H_{12}]$ (I) (S=0)**	**$[Rh_6(PH_3)_6H_{12}]$ (Calc) (S=1)**
Rh-Rh mean	2.741	2.712	2.716
Rh-Rh	2.739(1)-2.742(1)	2.709-2.718	2.707-2.732
δ(Rh-Rh) [a]	0.003	0.009	0.03
Rh···Rh cross-cluster	3.875	3.838	3.796-3.864
δ(Rh···Rh)	n/a	n/a	0.068
P···P cross-cluster	8.328	8.190	8.157-8.220
δ(P···P) [a]	n/a	n/a	0.063
Approx. Rh_6 vol.[b] / $Å^3$	9.7	9.4	9.5

[a] Maximum deviation in distances. [b] Calculated assuming a regular octahedron using the mean Rh-Rh distance.

Thermodynamic Data for Hydrogen Uptake and Release

Compound	Gas Energy[a]	ZPE[b]	TS[c]	E_{int}[d]	Solvent[e]	Total Energy[f]
$[Rh_6(PH_3)H_{12}]^{2+}$ (III)	-154.80	6.77	2.78	7.67	-4.99	-148.13
$Rh_6(PH_3)H_{16}]^{2+}$ (VII)	-169.60	7.43	2.68	7.51	-4.93	-162.37
$Rh_6(PH_3)H_{16}]^{+}$ (VI)	-178.01	7.31	2.82	8.25	-1.41	-166.68
$[Rh_6(PH_3)H_{12}]^{+}$ (II)	-163.63	6.66	2.82	7.58	-1.48	-153.69
$[Rh_6(PH_3)H_{14}]^{+}$ (IX)	-170.96	6.99	2.75	7.88	-1.47	-160.32
$[Rh_6(PH_3)H_{14}]^{2+}$ (X)	-162.24	7.09	2.75	7.98	-5.03	-154.96
H_2	-6.72	0.26	0.4	0.32	0.04	-6.5

[a] Gas phase SCF energy, [b] Zero point energy correction, [c] Entropy correction at 298.15K and 1atm, [d] Internal energy correction at 298.15K, [e] Solvent correction (CH_2Cl_2), [f] Total energy obtained by adding the correction factors to the gas phase SCF energies. All energies are in electron volts.

Optimized Geometries in the Gas Phase

$[Rh_6(PH_3)_6H_{12}]$ (I)

Rh	-1.054633	1.578020	-0.025057
Rh	1.167477	0.760686	-1.337172
Rh	1.102853	0.756611	1.394010
Rh	-1.167706	-0.761006	1.336955
Rh	-1.103091	-0.756734	-1.393813
Rh	1.054532	-1.578139	0.025227
P	2.287118	-3.375119	0.111577
H	3.665643	-3.333199	-0.274582
H	2.494961	-4.048269	1.358077
H	1.949111	-4.544663	-0.643110
H	2.026565	-0.752510	-1.207488
H	1.979398	-0.773396	1.278906
H	-0.079972	-2.144521	1.239482
H	-0.052482	-2.136617	-1.246899
P	-2.417395	-1.707818	-2.851523
H	-3.785530	-1.304536	-2.979305
H	-2.679778	-3.112767	-2.774881
H	-2.118459	-1.683416	-4.253628
H	-1.980377	0.772761	-1.277743
H	-2.074420	-1.390000	-0.206749
H	0.185720	0.093725	-2.496642
P	-2.427737	-1.514097	2.950433
H	-3.749696	-2.004715	2.691204
H	-2.793496	-0.654109	4.034249
H	-2.012310	-2.616427	3.764985
H	-2.026800	0.752195	1.207507
H	-0.185884	-0.094210	2.496542
P	2.417800	1.707743	2.851110
H	3.786244	1.305091	2.977571

H	2.679378	3.112868	2.775024
H	2.119995	1.682410	4.253447
H	2.073956	1.389783	0.206585
H	0.051963	2.136264	1.247628
P	2.427615	1.513988	-2.950460
H	3.749646	2.004405	-2.691162
H	2.793260	0.654125	-4.034432
H	2.012323	2.616511	-3.764837
H	0.079870	2.144128	-1.239528
P	-2.285626	3.375884	-0.112243
H	-3.663461	3.336362	0.276757
H	-2.495269	4.046925	-1.359596
H	-1.944840	4.546536	0.639496

$[Rh_6(PH_3)_6H_{12}]^+$ (II)

Rh	-0.033785	0.019406	-1.940147
P	0.031591	-0.094116	-4.124909
H	0.268314	1.133797	-4.818536
H	1.019266	-0.893307	-4.774521
H	-1.103971	-0.539969	-4.864180
H	0.009390	-1.543023	-2.130032
H	-1.787983	0.021041	-1.740973
Rh	0.027332	0.001310	1.950772
P	-0.022461	0.104576	4.143141
H	-0.380177	1.315282	4.807192
H	-0.926753	-0.769017	4.824141
H	1.156516	-0.190651	4.894384
H	0.043236	1.561390	2.126310
H	-1.710634	0.047716	1.776775
Rh	0.047196	-1.906495	-0.016259
P	-0.059694	-4.099060	0.032035
H	-0.528748	-4.765490	1.201878
H	-0.914012	-4.737955	-0.919809
H	1.116412	-4.883301	-0.183538
H	0.064607	-2.118808	1.535272
Rh	-0.037272	1.927706	0.023533
P	0.024155	4.117268	-0.075840
H	-0.010919	2.156842	-1.531000
H	0.140372	4.833470	1.155259
H	1.079425	4.757279	-0.790364
H	-1.066853	4.845012	-0.639240
Rh	1.885608	0.042728	-0.007999
P	4.076243	-0.071959	-0.001866
H	4.852936	1.114823	0.149967
H	4.725359	-0.862780	0.992237
H	4.749269	-0.604238	-1.144987

Rh	-1.874027	-0.010791	0.014604
P	-4.073879	-0.040187	0.037172
H	-1.805135	1.730661	0.011670
H	-4.797553	1.188567	0.074848
H	-4.777269	-0.650767	-1.047221
H	-4.749390	-0.701810	1.107463
H	-1.672989	-1.786346	0.058566
H	1.680633	1.834819	0.004887
H	1.814845	-1.690908	0.038865
H	1.773950	0.049002	1.746306
H	1.692500	0.027716	-1.780227

$[Rh_6(PH_3)_6H_{12}]^{2+}$ (III)

Rh	-0.054493	-0.007252	-1.923264
P	0.061623	-0.120388	-4.118088
H	0.293105	1.140807	-4.747539
H	1.095125	-0.892167	-4.722439
H	-1.054369	-0.580992	-4.876122
H	0.001131	-1.568644	-2.151310
H	-1.797610	-0.024181	-1.711285
Rh	0.057023	0.021281	1.940877
P	-0.034464	0.157416	4.142515
H	-0.460578	1.364503	4.766089
H	-0.935686	-0.759585	4.763561
H	1.146528	-0.095746	4.901734
H	0.015567	1.584170	2.136793
H	-1.692384	0.065887	1.798486
Rh	0.064377	-1.885011	-0.032881
P	0.012731	-4.099131	-0.044363
H	-0.444953	-4.785110	1.115240
H	-0.799356	-4.724357	-1.035527
H	1.252356	-4.771003	-0.263579
H	0.101183	-2.133268	1.514567
Rh	-0.070079	1.907486	0.045839
P	-0.017067	4.119436	-0.066891
H	-0.102587	2.108051	-1.511597
H	0.152793	4.826973	1.160127
H	0.999756	4.731292	-0.851472
H	-1.165376	4.782731	-0.592702
Rh	1.915731	0.040545	-0.035232
P	4.106625	-0.173274	0.044493
H	4.819187	1.051727	0.223643
H	4.684022	-0.952894	1.087298
H	4.804573	-0.711655	-1.075194
Rh	-1.909804	-0.028067	0.050225
P	-4.115987	0.107702	-0.008330

H	-2.129853	1.536523	0.067639
H	-4.757182	1.378286	0.011999
H	-4.773470	-0.472927	-1.133218
H	-4.821023	-0.530578	1.056169
H	-1.489994	-2.134515	0.015807
H	1.485625	2.141866	0.014544
H	2.128514	-1.529726	-0.059283
H	1.802696	0.069592	1.725820
H	1.699682	-0.007744	-1.780711

$[Rh_6(PH_3)_6H_{12}]^{3+}$ (IV)

Rh -0.045218 0.014592 -1.908365
P 0.084064 -0.137572 -4.126583
H 0.319955 1.116879 -4.765470
H 1.110413 -0.948377 -4.687417
H -1.070924 -0.615492 -4.812114
H -0.036399 -1.544008 -2.141644
H -1.969457 -0.021597 -1.578511
Rh 0.054349 0.000887 1.925283
P -0.049426 0.153783 4.151117
H -0.690334 1.287021 4.726016
H -0.747142 -0.918878 4.783289
H 1.202061 0.148388 4.837013
H 0.036938 1.555742 2.144187
H -1.580635 0.032542 1.988032
Rh 0.049449 -1.906923 -0.035405
P -0.040052 -4.139693 -0.016653
H -0.716911 -4.776987 1.060251
H -0.670431 -4.738459 -1.147277
H 1.228490 -4.792480 0.006502
H 0.084925 -2.192319 1.504837
Rh -0.054351 1.922845 0.035825
P -0.002913 4.157193 -0.071723
H -0.082087 2.166624 -1.515617
H 0.265662 4.817109 1.163815
H 0.946407 4.765475 -0.938409
H -1.215933 4.778937 -0.490491
Rh 1.904503 0.045378 -0.036288
P 4.128860 -0.112177 0.031765
H 4.787814 1.143591 0.193881
H 4.712331 -0.884937 1.074383
H 4.776500 -0.645637 -1.119967
Rh -1.898157 -0.031140 0.057558
P -4.130302 0.081756 0.000304
H -2.143383 1.525220 0.064226
H -4.755711 1.359335 -0.037185

H -4.770201 -0.576607 -1.089339
H -4.767518 -0.516063 1.129088
H -1.494543 -2.171594 0.042893
H 1.489541 2.197325 -0.018093
H 2.146865 -1.514430 -0.042567
H 1.985234 0.052296 1.597711
H 1.591348 0.005558 -1.955024

$[Rh_6(PH_3)_6H_{12}]^{4+}$ (V)
Rh -0.044483 0.043484 -1.924779
P 0.098134 -0.089931 -4.177242
H 0.357360 1.172515 -4.794203
H 1.097663 -0.940214 -4.728143
H -1.104358 -0.542335 -4.800168
H -0.007327 -1.500505 -2.197141
H -2.200908 -0.009192 -1.474474
Rh 0.045156 -0.026008 1.937848
P -0.070409 0.104405 4.198954
H -0.782478 1.201295 4.761287
H -0.676932 -1.031307 4.818051
H 1.216980 0.188168 4.813319
H 0.033164 1.517175 2.202422
H -1.493359 -0.003107 2.219047
Rh 0.048325 -1.921637 -0.008447
P -0.049617 -4.178999 0.043069
H -0.794103 -4.793844 1.088184
H -0.612943 -4.747280 -1.141462
H 1.237444 -4.789748 0.143520
H 0.063798 -2.234632 1.528706
Rh -0.047700 1.936167 0.005894
P 0.006946 4.194404 -0.112645
H -0.047124 2.199996 -1.535288
H 0.290893 4.809502 1.145218
H 0.949603 4.794784 -0.994174
H -1.234025 4.777899 -0.509711
Rh 1.917032 0.038909 -0.040510
P 4.177705 -0.087220 0.024282
H 4.804297 1.183228 0.208258
H 4.757358 -0.893866 1.043809
H 4.768991 -0.595595 -1.171787
Rh -1.907301 -0.028303 0.062828
P -4.175507 0.070876 0.009026
H -2.195537 1.506941 0.052728
H -4.774678 1.357811 -0.106929
H -4.804196 -0.672700 -1.033981
H -4.752638 -0.462483 1.203468

H -1.490515 -2.189086 0.074077
H 1.487894 2.219728 -0.057682
H 2.206865 -1.495734 -0.023749
H 2.217268 0.027253 1.493507
H 1.499453 0.033807 -2.189257

$[Rh_6(PH_3)_6H_{16}]^+$ (VI)

Rh	-0.079285	-0.010881	-0.036465
Rh	2.756990	-0.053177	0.086239
Rh	2.483238	2.737499	0.025703
Rh	1.215442	1.290561	2.080182
P	0.334234	0.865515	4.072294
H	-1.080341	0.719964	4.211064
H	0.710350	-0.333877	4.750918
H	0.538515	1.769099	5.157571
H	-0.140843	2.504380	1.750894
H	2.259607	2.264746	2.858686
H	1.277785	1.343365	0.109107
H	0.043522	0.012862	1.712452
Rh	-0.297997	2.687835	-0.128230
P	-1.785992	4.206531	-0.709314
H	-2.463844	4.002954	-1.945642
H	-2.922418	4.436140	0.120589
H	-1.395240	5.566357	-0.901839
H	1.082624	3.799938	-0.159688
H	-1.336748	1.279971	-0.171757
H	-0.714828	3.251578	1.387335
Rh	1.242531	1.267298	-1.916355
P	1.625759	1.253130	-4.079742
H	1.030054	2.253210	-4.908129
H	1.197862	0.101708	-4.807377
H	2.952827	1.335659	-4.601326
H	2.408971	2.497053	-1.754205
H	-0.120793	2.457812	-1.812487
P	3.997827	4.368511	0.100504
H	4.747584	4.671584	-1.079549
H	3.633322	5.713463	0.422199
H	5.113633	4.280707	0.989557
H	2.445803	2.630161	1.828676
P	4.819462	-0.810978	0.208604
H	5.736597	-0.160273	1.085233
H	5.628974	-0.814612	-0.968069
H	5.056011	-2.153268	0.624425
H	1.320451	-1.142401	0.041600
H	2.397722	-1.617893	-0.093756
H	2.533039	0.101104	1.808859

H	3.686988	1.476884	0.084681
H	2.538916	0.163570	-1.745283
P	-1.143151	-1.923523	0.318303
H	-0.700480	-2.882488	1.281695
H	-1.296342	-2.821368	-0.781440
H	-2.513245	-1.872259	0.722233
H	-0.044827	-0.005881	-1.781828

$[Rh_6(PH_3)_6H_{16}]^{2+}$ (VII)

Rh	0.000021	-0.000252	0.000069
Rh	2.828887	0.000105	-0.000235
Rh	2.481202	2.769449	0.000277
Rh	1.359652	1.294342	2.117513
P	0.795553	0.473073	4.105222
H	-0.584022	0.469939	4.468180
H	1.099597	-0.900829	4.334833
H	1.349862	1.038722	5.287633
H	-0.055374	2.577981	1.870486
H	2.239656	2.242804	3.034755
H	1.254362	1.356577	0.117647
H	0.086827	0.031083	1.705651
Rh	-0.249734	2.744289	0.017441
P	-1.963707	3.990724	-0.614715
H	-2.746917	3.491187	-1.692922
H	-2.986597	4.283414	0.331230
H	-1.664447	5.300217	-1.091943
H	1.174073	3.898584	-0.014734
H	-1.218019	1.333955	-0.008597
H	-0.709235	3.222394	1.574318
Rh	1.250720	1.370390	-1.879525
P	1.409154	1.453475	-4.081473
H	0.858436	2.587738	-4.745397
H	0.793139	0.398858	-4.814585
H	2.712664	1.434578	-4.652064
H	2.365314	2.647090	-1.854893
H	-0.097765	2.606010	-1.664392
P	4.007997	4.246962	0.644809
H	4.779132	4.832106	-0.404691
H	3.573324	5.424391	1.319351
H	5.054891	3.844066	1.524297
H	2.455089	2.655438	1.747881
P	4.903495	-0.770524	0.089163
H	5.781926	-0.199731	1.053989
H	5.698074	-0.621491	-1.085782
H	5.111528	-2.152997	0.358018
H	1.446252	-1.161279	-0.027314

H	2.417857	-1.588136	-0.067425
H	2.663003	0.160289	1.715509
H	3.726932	1.488285	-0.014163
H	2.513877	0.249514	-1.828827
P	-1.235098	-1.813148	0.388846
H	-0.782068	-2.809649	1.302505
H	-1.545621	-2.642754	-0.729619
H	-2.548025	-1.607590	0.908347
H	0.054480	0.065503	-1.780611

$[Rh_6(PH_3)_6H_{14}]$ ($VIII_{Int}$)

Rh	0.133535	0.156201	0.049355
Rh	2.830352	-0.059602	0.036067
Rh	1.661439	2.392975	0.041201
P	1.779569	4.484610	0.665178
H	1.823567	5.524185	-0.314965
H	2.887949	4.952522	1.442689
H	0.755492	5.071057	1.477660
H	0.313209	1.674191	0.968972
H	2.865644	1.385081	0.987468
H	0.577400	3.008583	-1.117126
Rh	1.376795	-0.817048	-2.187919
P	1.469537	-2.021598	-3.999929
H	2.518715	-2.977800	-4.208595
H	0.396369	-2.892401	-4.387945
H	1.598154	-1.382289	-5.274998
H	0.172016	0.062098	-3.059189
Rh	0.158145	1.735395	-2.377929
P	-1.569926	3.052970	-2.528080
H	-2.201700	3.476416	-1.318261
H	-1.469525	4.346874	-3.132664
H	-2.760120	2.656409	-3.218280
H	1.719801	2.318935	-3.057371
Rh	3.011313	1.558172	-2.206015
P	4.130643	1.962374	-4.026761
H	3.589134	1.576856	-5.295745
H	5.431860	1.398106	-4.248321
H	4.480021	3.296164	-4.427489
H	2.708169	0.020531	-2.938555
H	2.969308	2.893422	-0.947628
H	0.054392	1.835171	-3.932098
H	0.132128	-1.259435	-0.925974
P	4.399959	-1.022108	1.204761
H	4.060564	-1.943197	2.244757
H	5.314968	-0.227981	1.963205
H	5.376589	-1.841725	0.557304

H	2.622079	-1.443783	-1.021964
H	4.037395	0.605364	-1.019167
P	-1.764260	-0.716155	0.702071
H	-1.776627	-1.901982	1.504328
H	-2.681765	0.034406	1.506075
H	-2.717920	-1.161814	-0.264098
H	-0.878982	0.924114	-1.091566
H	1.481149	-0.602900	1.004175
H	1.510086	0.848096	-1.118856

$[Rh_6(PH_3)_6H_{14}]$ (VIII)

Rh	1.188250	1.401641	-1.977401
Rh	-0.020297	0.109382	-0.018912
Rh	2.750744	-0.053800	-0.148690
Rh	2.565676	2.717148	-0.154112
Rh	-0.058072	2.758401	0.010246
P	-1.614690	4.253243	0.378810
H	-2.552475	4.590935	-0.649762
H	-2.587520	4.072098	1.413180
H	-1.274801	5.599647	0.726058
H	1.249560	3.916723	-0.107041
H	-0.039165	2.636387	-1.764817
H	0.214051	2.631036	1.713366
H	-1.197232	1.482972	0.069424
P	4.326486	3.973430	0.208822
H	5.179768	4.344155	-0.881390
H	4.174040	5.296386	0.736713
H	5.382748	3.585519	1.095636
H	2.384885	2.651136	-1.943204
H	3.703362	1.456949	-0.277316
H	2.549536	2.690592	1.573435
P	4.798332	-0.795180	0.039457
H	5.697509	-0.197728	0.978717
H	5.697182	-0.762789	-1.076325
H	5.065128	-2.149833	0.406245
H	1.246991	-1.059792	-0.097104
H	2.410775	-1.603049	-0.281055
H	2.622714	0.091041	1.608823
Rh	1.472956	1.371588	2.004407
P	0.608435	1.010448	3.977354
H	-0.812966	0.914443	4.110267
H	0.919319	-0.144237	4.767089
H	0.810560	1.961079	5.025838
H	0.215177	0.111069	1.651408
H	2.681621	1.768672	2.921491
P	-1.243164	-1.659555	0.406482

H	-0.857241	-2.666193	1.350406
H	-1.577859	-2.574472	-0.644813
H	-2.581429	-1.512437	0.899276
H	-0.036687	0.189571	-1.817829
P	1.167122	1.322222	-4.171085
H	0.439738	2.295033	-4.928152
H	0.664898	0.177086	-4.866515
H	2.386050	1.428874	-4.912985
H	2.429155	0.165070	-1.896046

$[Rh_6(PH_3)_6H_{14}]^+$ (IX_{Int})

Rh	0.094893	0.068823	-0.033270
Rh	2.857114	-0.026348	-0.000996
Rh	1.586574	2.336647	0.017168
P	1.526272	4.346700	0.900185
H	1.621264	5.483603	0.045090
H	2.538572	4.705464	1.840980
H	0.378079	4.742528	1.652767
H	0.132080	1.427355	0.928148
H	2.811251	1.457314	0.969950
H	0.424583	2.989747	-1.061003
Rh	1.498405	-0.760130	-2.202856
P	1.109895	-2.186486	-3.829953
H	1.842627	-3.414487	-3.841122
H	-0.201928	-2.725277	-3.989462
H	1.331428	-1.801786	-5.188225
H	0.291525	0.111567	-3.127052
Rh	0.101576	1.719367	-2.348849
P	-1.192371	3.400647	-2.923240
H	-2.220974	3.814418	-2.023170
H	-0.597905	4.679932	-3.144380
H	-1.976563	3.339017	-4.111475
H	1.614538	2.250126	-3.168265
Rh	2.975006	1.596899	-2.269918
P	4.328923	2.035067	-3.922643
H	3.864798	1.887595	-5.263872
H	5.534155	1.277063	-4.040992
H	4.890306	3.346389	-4.043368
H	2.863339	0.181727	-3.116706
H	2.851378	2.936973	-0.831494
H	-0.488434	1.092640	-3.677003
H	0.288686	-1.397739	-1.225740
P	4.408920	-1.045018	1.169019
H	4.035031	-2.150246	1.989972
H	5.139415	-0.291189	2.135092
H	5.507753	-1.644893	0.486287

H	2.743671	-1.403140	-1.014471
H	4.015711	0.687110	-1.106789
P	-1.547618	-0.695064	1.198038
H	-1.337099	-0.782638	2.607157
H	-2.814213	-0.037395	1.217940
H	-2.008892	-2.027818	0.968088
H	-0.973772	0.893085	-1.152649
H	1.447628	-0.616342	0.897448
H	1.491629	0.853472	-1.166425

$[Rh_6(PH_3)_6H_{14}]^+$ (IX)

Rh	1.204846	1.395053	-1.931109
Rh	-0.011025	0.077890	0.025731
Rh	2.771179	-0.053687	-0.173445
Rh	2.573705	2.693342	-0.046723
Rh	-0.046648	2.699488	0.048900
P	-1.631127	4.220933	0.270830
H	-2.682140	4.263493	-0.693350
H	-2.442999	4.253630	1.444908
H	-1.274448	5.602651	0.240578
H	1.264063	3.871354	0.024505
H	-0.056001	2.642626	-1.680617
H	0.183597	2.561683	1.780557
H	-1.196225	1.437351	0.107048
P	4.303011	4.061554	0.011975
H	5.055301	4.281170	-1.182690
H	4.087843	5.427913	0.363905
H	5.400185	3.809751	0.888902
H	2.358463	2.578478	-1.952728
H	3.734904	1.436604	-0.194444
H	2.672341	2.689846	1.599803
P	4.813850	-0.889030	-0.168753
H	5.845687	-0.240822	0.574615
H	5.509049	-0.997083	-1.411337
H	5.047817	-2.215245	0.297734
H	1.281211	-1.084612	-0.105684
H	2.392847	-1.607583	-0.248438
H	2.719165	0.051055	1.611019
Rh	1.390721	1.324663	2.003514
P	0.684447	1.488354	4.085725
H	-0.708392	1.729413	4.269307
H	0.821970	0.379669	4.970240
H	1.190258	2.505502	4.953118
H	0.291950	0.063184	1.861215
H	2.506794	0.291983	2.622519
P	-1.299090	-1.714328	0.139102

H	-1.061863	-2.730639	1.115360
H	-1.432861	-2.571497	-0.993732
H	-2.690571	-1.524985	0.400943
H	-0.111450	0.071600	-1.646497
P	1.220133	1.482606	-4.127609
H	0.602849	2.604383	-4.758255
H	0.581801	0.445011	-4.873448
H	2.459832	1.506187	-4.832249
H	2.442329	0.203481	-1.910017

$[Rh_6(PH_3)_6H_{14}]^{2+}$ (X_{Int})

Rh	0.125705	0.007763	0.006911
Rh	2.862674	-0.028497	-0.019345
Rh	1.614006	2.329312	0.031479
P	1.464776	4.311418	0.984836
H	1.511572	5.478751	0.171322
H	2.465224	4.635256	1.946858
H	0.279867	4.574492	1.737252
H	0.213676	1.059000	1.169451
H	2.817888	1.456925	0.979021
H	0.497412	3.008134	-1.100494
Rh	1.566109	-0.769016	-2.248899
P	1.008065	-2.275268	-3.758514
H	1.505584	-3.595438	-3.548239
H	-0.369106	-2.562904	-3.978060
H	1.430662	-2.048428	-5.103759
H	0.316171	0.120333	-3.115715
Rh	0.161285	1.715986	-2.330955
P	-1.305922	3.266808	-2.925880
H	-2.207956	3.736799	-1.926402
H	-0.804239	4.520419	-3.385473
H	-2.237593	2.996539	-3.967061
H	1.686401	2.208827	-3.128201
Rh	3.040013	1.562363	-2.248691
P	4.072560	2.294676	-4.045564
H	3.551098	1.963175	-5.327848
H	5.433610	1.905314	-4.220105
H	4.183897	3.712152	-4.177404
H	3.343043	0.230755	-3.025495
H	2.879419	3.046564	-0.549430
H	-0.396017	1.111898	-3.687040
H	0.586621	-1.693229	-1.444866
P	4.390367	-1.099324	1.190172
H	3.978626	-2.252831	1.914665
H	5.021857	-0.351801	2.224770
H	5.528671	-1.613135	0.508044

H	2.776387	-1.404791	-1.033623
H	4.085637	0.674844	-1.041301
P	-1.787377	-0.282875	1.044043
H	-1.737841	-0.738681	2.394502
H	-2.683384	0.814101	1.186567
H	-2.665206	-1.252574	0.470339
H	-0.867270	0.886797	-1.099116
H	1.555768	-0.673217	0.924305
H	1.524287	0.840780	-1.161494

$[Rh_6(PH_3)_6H_{14}]^{2+}$ (X)

Rh	1.202238	1.393880	-1.919393
Rh	-0.006101	0.022149	0.039063
Rh	2.795750	-0.045818	-0.163042
Rh	2.590503	2.663708	-0.023000
Rh	-0.050375	2.669934	0.061940
P	-1.694013	4.151497	0.182630
H	-2.653512	4.157635	-0.870726
H	-2.574533	4.112679	1.303056
H	-1.345894	5.534106	0.199222
H	1.311348	3.823982	0.082516
H	-0.061887	2.667343	-1.656866
H	0.080835	2.527219	1.805501
H	-1.168613	1.384003	0.033525
P	4.181139	4.196660	0.041667
H	4.627944	4.679316	-1.224952
H	3.892913	5.430172	0.691805
H	5.433417	3.892338	0.647910
H	2.296569	2.503882	-2.144783
H	3.787484	1.381179	-0.138485
H	2.897780	2.752038	1.527892
P	4.798941	-1.027459	-0.206034
H	5.862496	-0.437078	0.535459
H	5.438295	-1.140753	-1.475110
H	4.935591	-2.372418	0.238587
H	1.343477	-1.131958	-0.101673
H	2.346562	-1.606503	-0.232213
H	2.742763	0.059792	1.579031
Rh	1.357594	1.364795	2.012443
P	0.984333	1.637785	4.183575
H	-0.344627	1.955053	4.580639
H	1.263218	0.568843	5.079460
H	1.705831	2.695251	4.813706
H	0.300640	0.243416	2.276952
H	2.478408	0.281137	2.554838
P	-1.476085	-1.629471	-0.113509

H	-1.875805	-2.234265	1.116862
H	-1.173498	-2.799409	-0.867702
H	-2.755852	-1.325749	-0.661632
H	-0.091112	-0.230125	-1.514667
P	1.268453	1.528722	-4.122830
H	0.858717	2.750556	-4.730603
H	0.447054	0.601825	-4.832168
H	2.510007	1.324703	-4.788662
H	2.454418	0.259154	-1.915735

$[Rh_6(PH_3)_6H_{12}]$ (I) with no unpaired electrons

Rh	-0.831350000	-1.232179000	22.493892000
Rh	-3.540187000	-1.217822000	22.560305000
Rh	-2.173541000	-3.394828000	23.424559000
Rh	-0.761177000	-1.829233000	25.140448000
Rh	-2.128629000	0.347553000	24.275906000
Rh	-3.469552000	-1.815584000	25.206828000
P	-4.942862000	-2.235177000	26.753593000
H	-6.220946000	-2.786176000	26.415862000
H	-4.650035000	-3.164809000	27.802968000
H	-5.445077000	-1.199913000	27.605456000
H	-4.630276000	-1.495775000	23.886143000
H	-3.387624000	-3.484046000	24.733655000
H	-2.115840000	-2.042000000	26.274302000
H	-3.345176000	-0.048834000	25.446348000
P	-2.070003000	2.450883000	24.833191000
H	-0.874225000	3.220338000	24.662286000
H	-2.308591000	2.843686000	26.189699000
H	-2.951067000	3.412921000	24.243696000
H	-0.914015000	0.436542000	22.968331000
H	-0.876425000	-0.072594000	25.408053000
H	-3.394611000	0.454193000	23.027427000
P	0.875675000	-2.201746000	26.524832000
H	1.848471000	-1.187127000	26.799718000
H	1.818626000	-3.247991000	26.268329000
H	0.635516000	-2.551085000	27.892981000
H	0.329071000	-1.551946000	23.813465000
H	-0.906873000	-3.500820000	24.673084000
P	-2.231097000	-5.498771000	22.869789000
H	-3.425896000	-6.269028000	23.044151000
H	-1.992042000	-5.899499000	21.515407000
H	-1.348800000	-6.456063000	23.465258000
H	-3.425453000	-2.975178000	22.292738000
H	-0.957262000	-2.998736000	22.254608000
P	-5.175883000	-0.847014000	21.174427000
H	-6.145194000	-1.863730000	20.895398000

H	-6.123816000	0.196418000	21.425409000
H	-4.930477000	-0.497770000	19.807209000
H	-2.185596000	-1.004904000	21.426432000
P	0.642455000	-0.813860000	20.947223000
H	1.919150000	-0.258744000	21.283298000
H	0.344711000	0.114682000	19.898671000
H	1.147657000	-1.846426000	20.093816000

H_2

H	0.116811	0.000000	0.000000
H	0.883189	0.000000	0.000000