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Supporting Information

All calculations use the B3LYP method in the Gaussian94 Package.

The LANL2DZ basis set was used throughout except where stated otherwise.

[YH₂]⁺

Y -0.0445488498 0. -0.0353723253

H -0.0454253958 0. 1.8410374823

H 1.7828305373 0. -0.4615167962

SCF Done: E(RB+HF-LYP) = -38.8170512205 A.U. after 6 cycles

Frequencies -- 477.3115 1623.9972 1671.4251

Natural Population

Natural					
Atom No	Charge	Core	Valence	Rydberg	Total
Y 1	1.90981	35.97137	1.10682	0.01199	37.09019
H 2	-0.45491	0.00000	1.45486	0.00004	1.45491
H 3	-0.45491	0.00000	1.45486	0.00004	1.45491
* Total *	1.00000	35.97137	4.01655	0.01208	40.00000
Total non-Lewis 0.02940 (0.074% of 40)					
1. (1.99961) BD (1) Y 1- H 2					
(27.42%) 0.5237* Y 1 s(30.29%)p 0.03(1.04%)d 2.27(68.68%)					
2. (1.99961) BD (1) Y 1- H 3					
(27.42%) 0.5237* Y 1 s(30.29%)p 0.03(1.04%)d 2.27(68.68%)					

PtH₂

Pt -0.0190424741 0. -0.0206722989

H -0.0193774094 0. 1.5081740361

H 1.5046903862 0. 0.1042652806

SCF Done: E(RB+HF-LYP) = -120.327306996 A.U. after 8 cycles

Frequencies -- 845.8732 2344.1145 2389.1018

Natural Population

Natural					
Atom No	Charge	Core	Valence	Rydberg	Total
Pt 1	-0.16171	67.97872	10.17036	0.01263	78.16171
H 2	0.08085	0.00000	0.91756	0.00159	0.91915
H 3	0.08085	0.00000	0.91756	0.00159	0.91915
* Total *	0.00000	67.97872	12.00547	0.01581	80.00000

Total non-Lewis 0.09606 (0.120% of 80)
1. (1.96358) BD (1)Pt 1- H 2
(54.56%) 0.7387*Pt 1 s(44.41%)p 0.00(0.12%)d 1.25(55.47%)
2. (1.96358) BD (1)Pt 1- H 3
(54.56%) 0.7387*Pt 1 s(44.41%)p 0.00(0.12%)d 1.25(55.47%)

[ZrH₃]⁺

Zr 0. 0. 0.0539380383
H 0.8035165574 -1.3917315022 -0.7191738441
H 0.8035165574 1.3917315022 -0.7191738441
H -1.6070331149 0. -0.7191738441

SCF Done: E(RB+HF-LYP) = -47.9749662669 A.U. after 7 cycles
Frequencies -- 341.5555 384.8225 385.0560
Frequencies -- 1789.9858 1790.3481 1849.4416

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Zr 1	1.73959	35.95867	2.29595	0.00579	38.26041
H 2	-0.24653	0.00000	1.24637	0.00016	1.24653
H 3	-0.24653	0.00000	1.24637	0.00016	1.24653
H 4	-0.24653	0.00000	1.24637	0.00016	1.24653
* Total *	1.00000	35.95867	6.03506	0.00627	42.00000

Total non-Lewis 0.05585 (0.133% of 42)
1. (1.99516) BD (1)Zr 1- H 2
(37.86%) 0.6153*Zr 1 s(28.90%)p 0.01(0.23%)d 2.45(70.87%)
2. (1.99516) BD (1)Zr 1- H 3
(37.86%) 0.6153*Zr 1 s(28.90%)p 0.01(0.23%)d 2.45(70.87%)
3. (1.99516) BD (1)Zr 1- H 4
(37.86%) 0.6153*Zr 1 s(28.90%)p 0.01(0.23%)d 2.45(70.87%)

RhH₃

Rh 0. 0. 0.0609467414
H 0.5878313714 -1.0181538016 -0.9142011208
H 0.5878313714 1.0181538016 -0.9142011208
H -1.1756627428 0. -0.9142011208

SCF Done: E(RB+HF-LYP) = -111.261411341 A.U. after 9 cycles
Frequencies -- 784.8660 793.0506 829.6953
Frequencies -- 2208.9967 2210.4381 2284.4849

Natural Population					
Natural		-----			
Atom No	Charge	Core	Valence	Rydberg	Total
Rh 1	-0.18057	35.96910	9.19929	0.01218	45.18057
H 2	0.06019	0.00000	0.93892	0.00089	0.93981
H 3	0.06019	0.00000	0.93892	0.00089	0.93981
H 4	0.06019	0.00000	0.93892	0.00089	0.93981
* Total *	0.00000	35.96910	12.01604	0.01486	48.00000
Total non-Lewis		0.24360 (0.508% of 48)			
1. (1.92924) BD (1)Rh 1- H 2					
(53.56%) 0.7319*Rh 1 s(33.23%)p 0.01(0.26%)d 2.00(66.51%)					
2. (1.92924) BD (1)Rh 1- H 3					
(53.56%) 0.7319*Rh 1 s(33.23%)p 0.01(0.26%)d 2.00(66.51%)					
3. (1.92924) BD (1)Rh 1- H 4					
(53.56%) 0.7319*Rh 1 s(33.23%)p 0.01(0.26%)d 2.00(66.51%)					

[TaH₄]⁺ Td

Ta 0. 0. 0.

H 0.9891828978 -0.9891828978 0.9891828978

H 0.9891828978 0.9891828978 -0.9891828978

H -0.9891828978 -0.9891828978 -0.9891828978

H -0.9891828978 0.9891828978 0.9891828978

SCF Done: E(RB+HF-LYP) = -59.7775437841 A.U. after 6 cycles
 Frequencies -- 610.9002 610.9067 610.9099
 Frequencies -- 783.1116 783.1128 1893.6216
 Frequencies -- 1893.6231 1893.6231 1960.4346

		Natural Population			
Natural		-----			
Atom No	Charge	Core	Valence	Rydberg	Total
Ta 1	1.59682	67.95990	3.43409	0.00919	71.40318
H 2	-0.14921	0.00000	1.14914	0.00007	1.14921
H 3	-0.14921	0.00000	1.14914	0.00007	1.14921
H 4	-0.14921	0.00000	1.14914	0.00007	1.14921
H 5	-0.14921	0.00000	1.14914	0.00007	1.14921
* Total *	1.00000	67.95990	8.03064	0.00947	76.00000
Total non-Lewis		0.04365 (0.057% of 76)			
1. (1.99911) BD (1)Ta 1- H 2					
(42.75%) 0.6538*Ta 1 s(25.00%)p 0.01(0.26%)d 2.99(74.74%)					

2. (1.99911) BD (1)Ta 1- H 3
(42.75%) 0.6538*Ta 1 s(25.00%)p 0.01(0.26%)d 2.99(74.74%)
3. (1.99911) BD (1)Ta 1- H 4
(42.75%) 0.6538*Ta 1 s(25.00%)p 0.01(0.26%)d 2.99(74.74%)
4. (1.99911) BD (1)Ta 1- H 5
(42.75%) 0.6538*Ta 1 s(25.00%)p 0.01(0.26%)d 2.99(74.74%)

[TaH₅]⁺ C4v

Ta 0. 0. -0.049774647

H -1.4035994609 0. 0.9083873079

H 0. 1.4035994609 0.9083873079

H 1.4035994609 0. 0.9083873079

H 0. -1.4035994609 0.9083873079

SCF Done: E(RB+HF-LYP) = -59.7657267196 A.U. after 5 cycles

Frequencies -- 602.0499 602.0515 636.2496

Frequencies -- 857.7574 884.4268 1933.1477

Frequencies -- 1933.1480 1935.2499 1986.1068

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Ta 1	1.35216	67.95390	3.67992	0.01403	71.64784
H 2	-0.08804	0.00000	1.08721	0.00083	1.08804
H 3	-0.08804	0.00000	1.08721	0.00083	1.08804
H 4	-0.08804	0.00000	1.08721	0.00083	1.08804
H 5	-0.08804	0.00000	1.08721	0.00083	1.08804
* Total *	1.00000	67.95390	8.02874	0.01736	76.00000

Total non-Lewis 0.13561 (0.178% of 76)

1. (1.97763) BD (1)Ta 1- H 2
(45.79%) 0.6767*Ta 1 s(24.96%)p 0.01(0.32%)d 2.99(74.72%)
2. (1.97763) BD (1)Ta 1- H 3
(45.79%) 0.6767*Ta 1 s(24.96%)p 0.01(0.32%)d 2.99(74.72%)
3. (1.97763) BD (1)Ta 1- H 4
(45.79%) 0.6767*Ta 1 s(24.96%)p 0.01(0.32%)d 2.99(74.72%)
4. (1.97763) BD (1)Ta 1- H 5
(45.79%) 0.6767*Ta 1 s(24.96%)p 0.01(0.32%)d 2.99(74.72%)

RuH₄ Td

Ru 0. 0. 0.

H 0.9091871816 0.9091871816 0.9091871816
H 0.9091871816 -0.9091871816 -0.9091871816
H -0.9091871816 -0.9091871816 0.9091871816
H -0.9091871816 0.9091871816 -0.9091871816

SCF Done: E(RB+HF-LYP) = -96.1794259984 A.U. after 9 cycles
Frequencies -- 750.4925 750.4934 750.4948
Frequencies -- 930.7519 930.7519 2099.0967
Frequencies -- 2099.0967 2099.0971 2122.8240

Natural Population

Atom No	Natural Charge	Core	Valence	Rydberg	Total
Ru 1	-0.18539	35.95742	8.21932	0.00864	44.18539
H 2	0.04635	0.00000	0.95355	0.00011	0.95365
H 3	0.04635	0.00000	0.95355	0.00011	0.95365
H 4	0.04635	0.00000	0.95355	0.00011	0.95365
H 5	0.04635	0.00000	0.95355	0.00011	0.95365
* Total *	0.00000	35.95742	12.03351	0.00907	48.00000

Total non-Lewis 0.09861 (0.205% of 48)

- (1.98599) BD (1)Ru 1- H 2
(52.64%) 0.7255*Ru 1 s(25.00%)p 0.00(0.10%)d 3.00(74.90%)
- (1.98599) BD (1)Ru 1- H 3
(52.64%) 0.7255*Ru 1 s(25.00%)p 0.00(0.10%)d 3.00(74.90%)
- (1.98599) BD (1)Ru 1- H 4
(52.64%) 0.7255*Ru 1 s(25.00%)p 0.00(0.10%)d 3.00(74.90%)
- (1.98599) BD (1)Ru 1- H 5
(52.64%) 0.7255*Ru 1 s(25.00%)p 0.00(0.10%)d 3.00(74.90%)

RuH₄ C_{4v}

Ru 0. 0. -0.0786617287
H -1.2424319265 0. 0.8652790156
H 0. 1.2424319265 0.8652790156
H 1.2424319265 0. 0.8652790156
H 0. -1.2424319265 0.8652790156

SCF Done: E(RB+HF-LYP) = -96.1930667392 A.U. after 9 cycles
Frequencies -- 693.5840 693.5915 774.4407
Frequencies -- 1024.2023 1026.2074 2134.1670
Frequencies -- 2192.2633 2192.2642 2223.3155

Natural Population

Natural -----					
Atom No	Charge	Core	Valence	Rydberg	Total
Ru 1	-0.32563	35.95885	8.35304	0.01374	44.32563
H 2	0.08141	0.00000	0.91751	0.00108	0.91859
H 3	0.08141	0.00000	0.91751	0.00108	0.91859
H 4	0.08141	0.00000	0.91751	0.00108	0.91859
H 5	0.08141	0.00000	0.91751	0.00108	0.91859
* Total *	0.00000	35.95885	12.02308	0.01806	48.00000
Total non-Lewis 0.38214 (0.796% of 48)					

1. (1.91480) BD (1)Ru 1- H 2
(54.79%) 0.7402*Ru 1 s(24.98%)p 0.01(0.23%)d 2.99(74.79%)
2. (1.91480) BD (1)Ru 1- H 3
(54.79%) 0.7402*Ru 1 s(24.98%)p 0.01(0.23%)d 2.99(74.79%)
3. (1.91480) BD (1)Ru 1- H 4
(54.79%) 0.7402*Ru 1 s(24.98%)p 0.01(0.23%)d 2.99(74.79%)
4. (1.91480) BD (1)Ru 1- H 5
(54.79%) 0.7402*Ru 1 s(24.98%)p 0.01(0.23%)d 2.99(74.79%)

[WH₅]⁺ (C4v, 1)

W -0.0121932116 0.0375262977 -0.0506977372
H 0.2958618531 -0.9105691545 1.2301200075
H 0.8618668986 0.597530867 1.2472425956
H -1.0484847993 -0.0231800263 1.2472425956
H 1.3517210176 -0.9100246538 0.0134972511
H -0.5586662042 -1.5307470896 0.0134972511

SCF Done: E(RB+HF-LYP) = -70.3388035328 A.U. after 9 cycles
Frequencies -- 351.6173 351.6261 764.1240
Frequencies -- 972.9673 1097.8539 1097.8565
Frequencies -- 1162.8041 2000.6175 2016.0113
Frequencies -- 2016.0123 2047.4792 2106.3762

Natural Population

Natural -----					
Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.71737	67.95135	5.31402	0.01726	73.28263
H 2	0.15447	0.00000	0.84350	0.00204	0.84553
H 3	0.03204	0.00000	0.96659	0.00137	0.96796
H 4	0.03204	0.00000	0.96659	0.00137	0.96796
H 5	0.03204	0.00000	0.96659	0.00137	0.96796

H 6	0.03204	0.00000	0.96659	0.00137	0.96796
* Total *	1.00000	67.95135	10.02388	0.02477	78.00000

Total non-Lewis 0.37075 (0.475% of 78)

- (1.85733) BD (1) W 1- H 2
(57.82%) 0.7604* W 1 s(16.83%)p 0.01(0.10%)d 4.94(83.07%)
- (1.95517) BD (1) W 1- H 3
(52.30%) 0.7232* W 1 s(20.79%)p 0.01(0.29%)d 3.80(78.91%)
- (1.95517) BD (1) W 1- H 4
(52.30%) 0.7232* W 1 s(20.79%)p 0.01(0.29%)d 3.80(78.91%)
- (1.95518) BD (1) W 1- H 5
(52.30%) 0.7232* W 1 s(20.79%)p 0.01(0.29%)d 3.79(78.91%)
- (1.95518) BD (1)' W 1- H 6
(52.30%) 0.7232* W 1 s(20.79%)p 0.01(0.29%)d 3.79(78.91%)

[WH₅]⁺ (Cs, h)

W 0.0000000127 0.0251611519 0.

H -1.3105189873 1.0788041519 0.

H 0.9135270127 -0.1151518481 1.388427

H 0.9135270127 -0.1151518481 -1.388427

H -0.2582679873 -1.3552128481 0.871427

H -0.2582679873 -1.3552128481 -0.871427

SCF Done: E(RB+HF-LYP) = -70.3362467977 A.U. after 9 cycles

Frequencies --	414.3452	439.0790	880.4776
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Frequencies --	910.2788	941.4556	1040.7629
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Frequencies --	1066.0727	1886.6901	1890.2252
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Frequencies --	1977.5771	2003.3719	2006.1018
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Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.95518	67.94997	5.08340	0.01145	73.04482
H 2	-0.03695	0.00000	1.03678	0.00017	1.03695
H 3	-0.00525	0.00000	1.00453	0.00072	1.00525
H 4	-0.00525	0.00000	1.00453	0.00072	1.00525
H 5	0.04614	0.00000	0.95265	0.00121	0.95386
H 6	0.04614	0.00000	0.95265	0.00121	0.95386
* Total *	1.00000	67.94997	10.03454	0.01550	78.00000

Total non-Lewis 0.22606 (0.290% of 78)

1. (1.99824) BD (1) W 1- H 2

- (48.40%) 0.6957* W 1 s(19.66%)p 0.01(0.17%)d 4.08(80.17%)
2. (1.97141) BD (1) W 1- H 3
(50.13%) 0.7080* W 1 s(19.06%)p 0.01(0.21%)d 4.24(80.73%)
3. (1.97141) BD (1) W 1- H 4
(50.13%) 0.7080* W 1 s(19.06%)p 0.01(0.21%)d 4.24(80.73%)
4. (1.94148) BD (1) W 1- H 5
(52.59%) 0.7252* W 1 s(18.59%)p 0.01(0.12%)d 4.37(81.28%)
5. (1.94148) BD (1) W 1- H 6
(52.59%) 0.7252* W 1 s(18.59%)p 0.01(0.12%)d 4.37(81.28%)

[WH₅]⁺ (Cs, g)

W -0.0341851949 -0.0346416471 0.0026418084
H 1.1162943261 0.8452655804 0.7804583746
H -0.6365700482 0.7223824244 -1.3611996058
H -0.5067660307 0.8029174313 1.3705531367
H 1.0349072621 0.7952595579 -0.9307566621
H 1.5218389137 -0.6023431097 -0.0545490637

SCF Done: E(RB+HF-LYP) = -70.3345036451 A.U. after 10 cycles

Frequencies --	317.8854	423.6797	876.6073
Frequencies --	923.2747	932.6016	1059.4235
Frequencies --	1182.7645	1902.5025	1953.1680
Frequencies --	2005.1057	2015.9313	2051.3341

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.81700	67.94961	5.22048	0.01291	73.18300
H 2	0.09433	0.00000	0.90419	0.00149	0.90567
H 3	-0.00792	0.00000	1.00704	0.00088	1.00792
H 4	-0.00794	0.00000	1.00705	0.00088	1.00794
H 5	0.09432	0.00000	0.90419	0.00149	0.90568
H 6	0.01021	0.00000	0.98871	0.00108	0.98979
* Total *	1.00000	67.94961	10.03167	0.01872	78.00000

Total non-Lewis 0.32081 (0.411% of 78)

1. (1.91634) BD (1) W 1- H 2
(55.06%) 0.7420* W 1 s(18.72%)p 0.00(0.08%)d 4.34(81.19%)
2. (1.97308) BD (1) W 1- H 3
(50.09%) 0.7077* W 1 s(20.52%)p 0.01(0.17%)d 3.87(79.31%)
3. (1.97308) BD (1) W 1- H 4

(50.09%) 0.7077* W 1 s(20.52%)p 0.01(0.17%)d 3.86(79.31%)
4. (1.91637) BD (1) W 1- H 5
(55.06%) 0.7420* W 1 s(18.73%)p 0.00(0.08%)d 4.34(81.19%)
5. (1.95080) BD (1) W 1- H 6
(51.11%) 0.7149* W 1 s(16.45%)p 0.02(0.31%)d 5.06(83.25%)

[WH₅]⁺ (C4v, j)

W 0. 0. 0.022877728

H 0. 0. 1.692469556

H 1.4220153859 0. -0.846355357

H 0. -1.4220153859 -0.846355357

H -1.4220153859 0. -0.846355357

H 0. 1.4220153859 -0.846355357

SCF Done: E(RB+HF-LYP) = -70.3346722328 A.U. after 9 cycles

Frequencies --	149.2138	149.3345	603.8269
Frequencies --	1012.5804	1019.1791	1019.1817
Frequencies --	1051.4657	1923.5480	1962.4064
Frequencies --	1962.4189	1976.0341	1996.6117

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.98649	67.95123	5.04984	0.01244	73.01351
H 2	-0.03393	0.00000	1.03385	0.00007	1.03393
H 3	0.01186	0.00000	0.98680	0.00134	0.98814
H 4	0.01186	0.00000	0.98680	0.00134	0.98814
H 5	0.01186	0.00000	0.98680	0.00134	0.98814
H 6	0.01186	0.00000	0.98680	0.00134	0.98814
* Total *	1.00000	67.95123	10.03090	0.01787	78.00000

Total non-Lewis 0.18975 (0.243% of 78)

1. (1.99921) BD (1) W 1- H 2
(48.52%) 0.6965* W 1 s(16.10%)p 0.01(0.14%)d 5.20(83.76%)
2. (1.96496) BD (1) W 1- H 3
(50.91%) 0.7135* W 1 s(20.96%)p 0.01(0.23%)d 3.76(78.80%)
3. (1.96496) BD (1) W 1- H 4
(50.91%) 0.7135* W 1 s(20.96%)p 0.01(0.23%)d 3.76(78.80%)
4. (1.96496) BD (1) W 1- H 5
(50.91%) 0.7135* W 1 s(20.96%)p 0.01(0.23%)d 3.76(78.80%)
5. (1.96496) BD (1) W 1- H 6

(50.91%) 0.7135* W 1 s(20.96%)p 0.01(0.23%)d 3.76(78.80%)

ReH₅ (C_{5v}, e)

Re 0. 0. 0.0480214463

H -1.4372938216 0. -0.7203216946

H -0.4441482168 -1.3669476549 -0.7203216946

H 1.1627951276 -0.8448201115 -0.7203216946

H -0.4441482168 1.3669476549 -0.7203216946

H 1.1627951276 0.8448201115 -0.7203216946

SCF Done: E(RB+HF-LYP) = -81.9506038870 A.U. after 10 cycles

Frequencies -- 487.0928 489.8172 908.0738

Frequencies -- 930.7543 935.2569 1184.9794

Frequencies -- 1185.7441 2076.3283 2076.8344

Frequencies -- 2077.9956 2078.3248 2116.4078

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	-0.12232	67.95659	7.14012	0.02561	75.12232
H 2	0.02446	0.00000	0.97416	0.00138	0.97554
H 3	0.02446	0.00000	0.97416	0.00138	0.97554
H 4	0.02446	0.00000	0.97416	0.00138	0.97554
H 5	0.02446	0.00000	0.97416	0.00138	0.97554
H 6	0.02446	0.00000	0.97416	0.00138	0.97554
* Total *	0.00000	67.95659	12.01092	0.03249	80.00000

Total non-Lewis 0.44149 (0.552% of 80)

1. (1.92040) BD (1)Re 1- H 2

(51.61%) 0.7184*Re 1 s(19.25%)p 0.01(0.27%)d 4.18(80.48%)

2. (1.92040) BD (1)Re 1- H 3

(51.61%) 0.7184*Re 1 s(19.25%)p 0.01(0.27%)d 4.18(80.48%)

3. (1.92040) BD (1)Re 1- H 4

(51.61%) 0.7184*Re 1 s(19.25%)p 0.01(0.27%)d 4.18(80.48%)

4. (1.92040) BD (1)Re 1- H 5

(51.61%) 0.7184*Re 1 s(19.25%)p 0.01(0.27%)d 4.18(80.48%)

5. (1.92040) BD (1)Re 1- H 6

(51.61%) 0.7184*Re 1 s(19.25%)p 0.01(0.27%)d 4.18(80.48%)

ReH₅ (C_s, g)

Re -0.0377224849 0.0121607743 0.

H 0.7090836297 1.4668543885 0.

H -0.2757803665 -0.7779393689 1.4327758087

H -0.2757803665 -0.7779393689 -1.4327758087

H 1.3358317371 -0.4115168631 0.7279583732

H 1.3358317371 -0.4115168631 -0.7279583732

SCF Done: E(RB+HF-LYP) = -81.9487274179 A.U. after 10 cycles

Frequencies -- 286.8013 369.1319 873.6375

Frequencies -- 937.7473 959.4628 1003.7199

Frequencies -- 1098.6922 2003.5331 2019.6587

Frequencies -- 2071.7484 2150.1608 2165.5259

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	-0.00934	67.95491	7.03138	0.02304	75.00934
H 2	-0.04384	0.00000	1.04313	0.00071	1.04384
H 3	-0.05648	0.00000	1.05575	0.00073	1.05648
H 4	-0.05648	0.00000	1.05575	0.00073	1.05648
H 5	0.08307	0.00000	0.91534	0.00160	0.91693
H 6	0.08307	0.00000	0.91534	0.00160	0.91693
* Total *	0.00000	67.95491	12.01669	0.02840	80.00000

Total non-Lewis 0.34243 (0.428% of 80)

1. (1.98755) BD (1)Re 1- H 2

(48.30%) 0.6950*Re 1 s(22.93%)p 0.02(0.53%)d 3.34(76.54%)

2. (1.97432) BD (1)Re 1- H 3

(47.73%) 0.6909*Re 1 s(18.97%)p 0.02(0.34%)d 4.25(80.70%)

3. (1.97432) BD (1)Re 1- H 4

(47.73%) 0.6909*Re 1 s(18.97%)p 0.02(0.34%)d 4.25(80.70%)

4. (1.88333) BD (1)Re 1- H 5

(54.37%) 0.7374*Re 1 s(19.41%)p 0.01(0.14%)d 4.15(80.45%)

5. (1.88333) BD (1)Re 1- H 6

(54.37%) 0.7374*Re 1 s(19.41%)p 0.01(0.14%)d 4.15(80.45%)

WH₆ (C3v, a)

W 0. 0. -0.0334202853

H -1.0156733339 0. 1.2892289467

H 0.5078366669 0.8795989091 1.2892289467

H 0.5078366669 -0.8795989091 1.2892289467

H -1.6499947178 0. -0.4648619088

H 0.8249973589 1.4289373417 -0.4648619088
H 0.8249973589 -1.4289373417 -0.4648619088

SCF Done: E(RB+HF-LYP) = -71.2761102438 A.U. after 8 cycles
Frequencies -- 701.7703 702.2319 806.5458
Frequencies -- 823.9042 954.1642 955.9407
Frequencies -- 987.5808 988.3563 1282.4625
Frequencies -- 1901.0163 1901.0549 1932.0158
Frequencies -- 2003.2198 2004.7537 2031.1811

Natural Population

Atom No	Natural Charge	Core	Valence	Rydberg	Total
W 1	0.39503	67.95271	5.63271	0.01955	73.60497
H 2	0.00138	0.00000	0.99644	0.00218	0.99862
H 3	0.00138	0.00000	0.99644	0.00218	0.99862
H 4	0.00138	0.00000	0.99644	0.00218	0.99862
H 5	-0.13306	0.00000	1.13227	0.00079	1.13306
H 6	-0.13306	0.00000	1.13227	0.00079	1.13306
H 7	-0.13306	0.00000	1.13227	0.00079	1.13306
* Total *	0.00000	67.95271	12.01883	0.02846	80.00000

Total non-Lewis 0.36352 (0.454% of 80)

- (1.91908) BD (1) W 1- H 2
(50.08%) 0.7077* W 1 s(13.72%)p 0.02(0.23%)d 6.27(86.05%)
- (1.91908) BD (1) W 1- H 3
(50.08%) 0.7077* W 1 s(13.72%)p 0.02(0.23%)d 6.27(86.05%)
- (1.91908) BD (1) W 1- H 4
(50.08%) 0.7077* W 1 s(13.72%)p 0.02(0.23%)d 6.27(86.05%)
- (1.97553) BD (1) W 1- H 5
(43.60%) 0.6603* W 1 s(19.63%)p 0.01(0.28%)d 4.08(80.09%)
- (1.97553) BD (1) W 1- H 6
(43.60%) 0.6603* W 1 s(19.63%)p 0.01(0.28%)d 4.08(80.09%)
- (1.97553) BD (1) W 1- H 7
(43.60%) 0.6603* W 1 s(19.63%)p 0.01(0.28%)d 4.08(80.09%)

WH₆ (C3v, b)

W 0. 0. -0.0554796616
H -1.0003038914 0. 1.2645947487
H 1.694808 0. 0.1039035699
H -0.847404 1.4677467826 0.1039035699

H 0.5001519457 -0.8662885815 1.2645947487

H 0.5001519457 0.8662885815 1.2645947487

H -0.847404 -1.4677467826 0.1039035699

SCF Done: E(RB+HF-LYP) = -71.2622660899 A.U. after 8 cycles

Frequencies -- 631.1364 795.5715 796.3262

Frequencies -- 807.6068 948.8001 949.4149

Frequencies -- 1188.7954 1189.0609 1223.7354

Frequencies -- 1927.0398 1927.4474 1937.3688

Frequencies -- 2051.6044 2053.4020 2077.7903

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.19145	67.94971	5.83521	0.02362	73.80855
H 2	0.05681	0.00000	0.94044	0.00275	0.94319
H 3	-0.12063	0.00000	1.11914	0.00149	1.12063
H 4	-0.12063	0.00000	1.11914	0.00149	1.12063
H 5	0.05681	0.00000	0.94044	0.00275	0.94319
H 6	0.05681	0.00000	0.94044	0.00275	0.94319
H 7	-0.12063	0.00000	1.11914	0.00149	1.12063
* Total *	0.00000	67.94971	12.01395	0.03635	80.00000
Total non-Lewis 0.44104 (0.551% of 80)					
1. (1.91100) BD (1) W 1- H 2					
(52.96%) 0.7278* W 1 s(15.17%)p 0.01(0.23%)d 5.58(84.60%)					
2. (1.95877) BD (1) W 1- H 3					
(44.33%) 0.6658* W 1 s(18.17%)p 0.02(0.43%)d 4.48(81.40%)					
3. (1.95877) BD (1) W 1- H 4					
(44.33%) 0.6658* W 1 s(18.17%)p 0.02(0.43%)d 4.48(81.40%)					
4. (1.91100) BD (1) W 1- H 5					
(52.96%) 0.7278* W 1 s(15.17%)p 0.01(0.23%)d 5.58(84.60%)					
5. (1.91100) BD (1) W 1- H 6					
(52.96%) 0.7278* W 1 s(15.17%)p 0.01(0.23%)d 5.58(84.60%)					
6. (1.95877) BD (1) W 1- H 7					
(44.33%) 0.6658* W 1 s(18.17%)p 0.02(0.43%)d 4.48(81.40%)					

WH₆ (C5v, c)

W 0. 0. -0.0217683842

H 0. 0. -1.7449132759

H 1.5291743509 0. 0.6711547408

H 0.4725408618 1.454331231 0.6711547408
H 0.4725408618 -1.454331231 0.6711547408
H -1.2371280372 0.8988261316 0.6711547408
H -1.2371280372 -0.8988261316 0.6711547408

SCF Done: E(RB+HF-LYP) = -71.2751880870 A.U. after 8 cycles

Frequencies --	680.5496	684.1860	763.8290
Frequencies --	764.4148	964.8248	965.1028
Frequencies --	1010.8789	1170.7912	1172.1188
Frequencies --	1865.0261	1950.6091	1950.9375
Frequencies --	1972.9260	1973.0226	2008.4225

Natural Population

Natural		-----			
Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.40859	67.95214	5.62190	0.01737	73.59141
H 2	-0.17478	0.00000	1.17464	0.00014	1.17478
H 3	-0.04676	0.00000	1.04530	0.00147	1.04676
H 4	-0.04676	0.00000	1.04530	0.00147	1.04676
H 5	-0.04676	0.00000	1.04530	0.00147	1.04676
H 6	-0.04676	0.00000	1.04530	0.00147	1.04676
H 7	-0.04676	0.00000	1.04530	0.00147	1.04676
* Total *	0.00000	67.95214	12.02302	0.02484	80.00000

Total non-Lewis 0.33062 (0.413% of 80)

1. (1.99968) BD (1) W 1- H 2
(41.42%) 0.6436* W 1 s(22.43%)p 0.01(0.25%)d 3.45(77.32%)
2. (1.94352) BD (1) W 1- H 3
(47.77%) 0.6912* W 1 s(15.52%)p 0.01(0.20%)d 5.43(84.28%)
3. (1.94352) BD (1) W 1- H 4
(47.77%) 0.6912* W 1 s(15.52%)p 0.01(0.20%)d 5.43(84.28%)
4. (1.94352) BD (1) W 1- H 5
(47.77%) 0.6912* W 1 s(15.52%)p 0.01(0.20%)d 5.43(84.28%)
5. (1.94352) BD (1) W 1- H 6
(47.77%) 0.6912* W 1 s(15.52%)p 0.01(0.20%)d 5.43(84.28%)
6. (1.94352) BD (1) W 1- H 7
(47.77%) 0.6912* W 1 s(15.52%)p 0.01(0.20%)d 5.43(84.28%)

WH₆ (C5v, d)

W 0. 0. -0.0621184643

H 0. 0. 1.584147125

H 1.5399897451 0. 0.602523847

H 0.4758830024 1.4646172821 0.602523847

H 0.4758830024 -1.4646172821 0.602523847

H -1.2458778749 0.9051832608 0.602523847

H -1.2458778749 -0.9051832608 0.602523847

SCF Done: E(RB+HF-LYP) = -71.2502561975 A.U. after 9 cycles

Frequencies -- 697.7906 703.0849 810.4180

Frequencies -- 811.0459 1076.3528 1149.7934

Frequencies -- 1150.4072 1208.7626 1210.9060

Frequencies -- 1965.3901 1965.4330 1996.8939

Frequencies -- 1997.1111 2016.7057 2116.9176

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.01413	67.94631	6.01650	0.02307	73.98587
H 2	0.14670	0.00000	0.85230	0.00100	0.85330
H 3	-0.03216	0.00000	1.02969	0.00247	1.03216
H 4	-0.03216	0.00000	1.02969	0.00247	1.03216
H 5	-0.03216	0.00000	1.02969	0.00247	1.03216
H 6	-0.03216	0.00000	1.02969	0.00247	1.03216
H 7	-0.03216	0.00000	1.02969	0.00247	1.03216
* Total *	0.00000	67.94631	12.01726	0.03643	80.00000

Total non-Lewis 0.46548 (0.582% of 80)

1. (1.92047) BD (1) W 1- H 2

(57.72%) 0.7597* W 1 s(18.33%)p 0.00(0.07%)d 4.45(81.61%)

2. (1.93356) BD (1) W 1- H 3

(48.68%) 0.6977* W 1 s(16.33%)p 0.02(0.34%)d 5.10(83.32%)

3. (1.93356) BD (1) W 1- H 4

(48.68%) 0.6977* W 1 s(16.33%)p 0.02(0.34%)d 5.10(83.32%)

4. (1.93356) BD (1) W 1- H 5

(48.68%) 0.6977* W 1 s(16.33%)p 0.02(0.34%)d 5.10(83.32%)

5. (1.93356) BD (1) W 1- H 6

(48.68%) 0.6977* W 1 s(16.33%)p 0.02(0.34%)d 5.10(83.32%)

6. (1.93356) BD (1) W 1- H 7

(48.68%) 0.6977* W 1 s(16.33%)p 0.02(0.34%)d 5.10(83.32%)

ZrH₄: (Td)

Zr 0. 0. 0.

H 1.0635747124 -1.0635747124 1.0635747124
H 1.0635747124 1.0635747124 -1.0635747124
H -1.0635747124 -1.0635747124 -1.0635747124
H -1.0635747124 1.0635747124 1.0635747124

SCF Done: E(RB+HF-LYP) = -48.8720238116 A.U. after 12 cycles
Frequencies -- 520.8079 520.8087 520.8093
Frequencies -- 629.6729 629.6735 1654.2351
Frequencies -- 1654.2357 1654.2361 1730.3822

Natural Population

Atom No	Natural Charge	Core	Valence	Rydberg	Total
Zr 1	1.46093	35.96338	2.55531	0.02038	38.53907
H 2	-0.36523	0.00000	1.36516	0.00007	1.36523
H 3	-0.36523	0.00000	1.36516	0.00007	1.36523
H 4	-0.36523	0.00000	1.36516	0.00007	1.36523
H 5	-0.36523	0.00000	1.36516	0.00007	1.36523
* Total *	0.00000	35.96338	8.01596	0.02066	44.00000

Total non-Lewis 0.03920 (0.089% of 44)

- (1.99936) BD (1)Zr 1- H 2
(31.87%) 0.5646*Zr 1 s(25.00%)p 0.03(0.82%)d 2.97(74.18%)
- (1.99936) BD (1)Zr 1- H 3
(31.87%) 0.5646*Zr 1 s(25.00%)p 0.03(0.82%)d 2.97(74.18%)
- (1.99936) BD (1)Zr 1- H 4
(31.87%) 0.5646*Zr 1 s(25.00%)p 0.03(0.82%)d 2.97(74.18%)
- (1.99936) BD (1)Zr 1- H 5
(31.87%) 0.5646*Zr 1 s(25.00%)p 0.03(0.82%)d 2.97(74.18%)

TaH₅: (C4v)

Ta 0. 0. 0.0196373288
H 0. 0. 1.7990770416
H 1.5358993588 0. -0.8081505114
H 0. -1.5358993588 -0.8081505114
H -1.5358993588 0. -0.8081505114
H 0. 1.5358993588 -0.8081505114

SCF Done: E(RB+HF-LYP) = -60.6851632667 A.U. after 12 cycles
Frequencies -- 289.9376 289.9612 752.3563
Frequencies -- 752.3593 838.4425 842.7331
Frequencies -- 905.7727 1764.4068 1819.2938

Frequencies -- 1855.1539 1855.1578 1902.7430

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Ta 1	1.23694	67.96112	3.77379	0.02816	71.76306
H 2	-0.32903	0.00000	1.32888	0.00015	1.32903
H 3	-0.22698	0.00000	1.22568	0.00130	1.22698
H 4	-0.22698	0.00000	1.22568	0.00130	1.22698
H 5	-0.22698	0.00000	1.22568	0.00130	1.22698
H 6	-0.22698	0.00000	1.22568	0.00130	1.22698
* Total *	0.00000	67.96112	10.00537	0.03351	78.00000

Total non-Lewis 0.14138 (0.181% of 78)

- (1.99432) BD (1)Ta 1- H 2
(33.56%) 0.5794*Ta 1 s(22.20%)p 0.03(0.72%)d 3.47(77.07%)
- (1.97580) BD (1)Ta 1- H 3
(38.57%) 0.6211*Ta 1 s(19.44%)p 0.04(0.75%)d 4.11(79.81%)
- (1.97580) BD (1)Ta 1- H 4
(38.57%) 0.6211*Ta 1 s(19.44%)p 0.04(0.75%)d 4.11(79.81%)
- (1.97580) BD (1)Ta 1- H 5
(38.57%) 0.6211*Ta 1 s(19.44%)p 0.04(0.75%)d 4.11(79.81%)
- (1.97580) BD (1)Ta 1- H 6
(38.57%) 0.6211*Ta 1 s(19.44%)p 0.04(0.75%)d 4.11(79.81%)

PtH₂ (Basis Set lacking 6p orbitals)

Pt -0.0188853012 0. -0.0204938845

H -0.0258515189 0. 1.5018000075

H 1.4989050099 0. 0.0967229796

SCF Done: E(RB+HF-LYP) = -120.325019474 A.U. after 7 cycles

Frequencies -- 848.4756 2440.6657 2475.7617

Basis set for this and for PtH₄ lacking p is LANL2DZ minus p orbitals;

H 0

LANL2DZ

Pt 0

S 3 1.00

0.254700D+01 -.147392D+01

0.161400D+01 0.191157D+01

0.516700D+00 0.392232D+00

```

S 4 1.00
0.254700D+01  0.143882D+01
0.161400D+01  -.209118D+01
0.516700D+00  -.109213D+01
0.265100D+00  0.134266D+01

S 1 1.00
0.580000D-01  0.100000D+01

P 3 1.00
0.291100D+01  -.524744D+00
0.183600D+01  0.967188D+00
0.598200D+00  0.543863D+00

!   P 2 1.00           (Gaussian ignores lines which begin with '!')
!0.604800D+00  -.106144D+00 (These were the LANL2DZ 6p-orbitals.)
!0.996000D-01  0.103831D+01 (The 3 primitive gaussian P orbital above
!   P 1 1.00           is the Pt's 5p orbital, so it is kept.)
!0.290000D-01  0.100000D+01

D 2 1.00
0.124300D+01  0.559815D+00
0.427100D+00  0.551109D+00

D 1 1.00
0.137000D+00  0.100000D+01
****

```

PT 0

LANL2DZ

\$end

		Natural Population			
Natural		-----			
Atom No	Charge	Core	Valence	Rydberg	Total
Pt 1	-0.17601	67.97541	10.19170	0.00890	78.17601
H 2	0.08800	0.00000	0.91004	0.00195	0.91200
H 3	0.08800	0.00000	0.91004	0.00195	0.91200
* Total *	0.00000	67.97541	12.01178	0.01281	80.00000
Total non-Lewis		0.09806 (0.123% of 80)			
1. (1.96437) BD (1)Pt 1- H 2					
(54.99%) 0.7416*Pt 1 s(44.43%)p 0.00(0.00%)d 1.25(55.57%)					
2. (1.96437) BD (1)Pt 1- H 3					

(54.99%) 0.7416*Pt 1 s(44.43%)p 0.00(0.00%)d 1.25(55.57%)

[ClF₂]⁺

Cl -0.4079446504 0. -0.4079446504

F -0.5613375907 0. 1.3318997081

F 1.3318997081 0. -0.5613375907

SCF Done: E(RB+HF-LYP) = -214.003406475 A.U. after 8 cycles

Frequencies -- 244.9795 653.8158 677.9467

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Cl 1	1.18285	10.00000	5.81186	0.00530	15.81715
F 2	-0.09142	2.00000	7.09017	0.00126	9.09142
F 3	-0.09142	2.00000	7.09017	0.00126	9.09142
* Total *	1.00000	13.99999	19.99219	0.00781	34.00000

Total non-Lewis 0.14214 (0.418% of 34)

1. (1.99739) BD (1)Cl 1- F 2

(43.52%) 0.6597*Cl 1 s(3.94%)p24.40(96.06%)

2. (1.99739) BD (1)Cl 1- F 3

(43.52%) 0.6597*Cl 1 s(3.94%)p24.40(96.06%)

[PtH₄]²⁺

Pt 0. 0. 0.

H 0. 0. 1.6938153775

H 1.6938153775 0. 0.

H -1.6938153775 0. 0.

H 0. 0. -1.6938153775

SCF Done: E(RB+HF-LYP) = -121.429579515 A.U. after 8 cycles

Frequencies -- 419.1933 443.3509 562.8689

Frequencies -- 562.8690 741.1097 1426.2793

Frequencies -- 1426.2793 1838.4202 1848.2612

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Pt 1	-0.56167	67.99764	10.29343	0.27060	78.56167
H 2	-0.35958	0.00000	1.35214	0.00744	1.35958
H 3	-0.35958	0.00000	1.35214	0.00744	1.35958
H 4	-0.35958	0.00000	1.35214	0.00744	1.35958

H 5 -0.35958 0.00000 1.35214 0.00744 1.35958
* Total * -2.00000 67.99764 15.70200 0.30036 84.00000

Atom No Natural Electron Configuration

Pt 1 [core]6s(0.98)5d(9.31)6p(0.27)
H 2 1s(1.35)2s(0.01)
H 3 1s(1.35)2s(0.01)
H 4 1s(1.35)2s(0.01)
H 5 1s(1.35)2s(0.01)

Total non-Lewis 1.36489 (1.625% of 84)

1. (1.96845) BD (1)Pt 1- H 2

(41.58%) 0.6448*Pt 1 s(42.18%)p 0.13(5.52%)d 1.24(52.30%)

2. (1.96845) BD (1)Pt 1- H 4

(41.58%) 0.6448*Pt 1 s(42.18%)p 0.13(5.52%)d 1.24(52.30%)

[RhH₄]⁻

Rh 0. 0. -0.047417002

H 0. 1.7020608991 -0.0123031236

H 1.0365132065 0. 1.0791856691

H -1.0365132065 0. 1.0791856691

H 0. -1.7020608991 -0.0123031236

SCF Done: E(RB+HF-LYP) = -111.880001564 A.U. after 9 cycles

Frequencies -- 340.7384 377.1028 682.1073

Frequencies -- 683.2407 765.2859 1424.9994

Frequencies -- 1724.2561 2180.3930 2230.5324

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Rh 1	-0.32258	35.97705	9.23806	0.10747	45.32258
H 2	-0.38596	0.00000	1.38071	0.00525	1.38596
H 3	0.04725	0.00000	0.95228	0.00047	0.95275
H 4	0.04725	0.00000	0.95228	0.00047	0.95275
H 5	-0.38596	0.00000	1.38071	0.00525	1.38596
* Total *	-1.00000	35.97705	13.90404	0.11891	50.00000

Total non-Lewis 0.79011 (1.580% of 50)

1. (1.94902) BD (1)Rh 1- H 3

(52.98%) 0.7279*Rh 1 s(27.66%)p 0.02(0.53%)d 2.60(71.81%)

2. (1.94902) BD (1)Rh 1- H 4

(52.98%) 0.7279*Rh 1 s(27.66%)p 0.02(0.53%)d 2.60(71.81%)

3. (1.95425) BD (1)Rh 1- H 5

(39.71%) 0.6302*Rh 1 s(40.96%)p 0.10(4.23%)d 1.34(54.81%)

ReH₆ (Cs, wide H'-Re-H')

Re 0.0227576488 -0.013702398 0.

H 1.5338460093 0.7522391017 0.

H -0.0599150224 1.6307852802 0.

H -0.8417794609 0.564240917 -1.2495233303

H -0.8417794609 0.564240917 1.2495233303

H -0.7485978612 -1.2419131815 -0.8412481419

H -0.7485978612 -1.2419131815 0.8412481419

SCF Done: E(UB+HF-LYP) = -82.5488402282 A.U. after 9 cycles

Frequencies --	215.5936	285.6134	598.5563
Frequencies --	688.6765	765.7504	777.6207
Frequencies --	989.5493	1054.8650	1058.5665
Frequencies --	1870.0254	1924.2278	1942.5307
Frequencies --	2030.4784	2077.1411	2120.6461

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	0.15213	67.96324	6.85700	0.02763	74.84787
H 2	-0.11869	0.00000	1.11521	0.00348	1.11869
H 3	-0.01638	0.00000	1.00999	0.00639	1.01638
H 4	0.05551	0.00000	0.94323	0.00126	0.94449
H 5	0.05551	0.00000	0.94323	0.00126	0.94449
H 6	-0.06404	0.00000	1.05860	0.00545	1.06404
H 7	-0.06404	0.00000	1.05860	0.00545	1.06404
* Total *	0.00000	67.96324	12.98585	0.05091	81.00000

***** Alpha spin orbitals *****

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	-0.43563	33.98270	3.93730	0.01563	37.93563
H 2	-0.06378	0.00000	0.56156	0.00222	0.56378
H 3	-0.00830	0.00000	0.50452	0.00378	0.50830
H 4	0.04229	0.00000	0.45710	0.00061	0.45771
H 5	0.04229	0.00000	0.45710	0.00061	0.45771

H 6	-0.03844	0.00000	0.53484	0.00359	0.53844
H 7	-0.03844	0.00000	0.53484	0.00359	0.53844
* Total *	-0.50000	33.98270	6.98726	0.03004	41.00000

Total non-Lewis 0.63650 (1.552% of 41)

1. (0.90625) BD (1)Re 1- H 2
(44.53%) 0.6673*Re 1 s(15.91%)p 0.95(15.19%)d 4.33(68.90%)
2. (0.83481) BD (1)Re 1- H 3
(47.04%) 0.6859*Re 1 s(15.43%)p 1.22(18.78%)d 4.26(65.78%)
3. (0.97014) BD (1)Re 1- H 4
(54.92%) 0.7411*Re 1 s(20.16%)p 0.01(0.20%)d 3.95(79.64%)
4. (0.97014) BD (1)Re 1- H 5
(54.92%) 0.7411*Re 1 s(20.16%)p 0.01(0.20%)d 3.95(79.64%)
5. (0.85085) BD (1)Re 1- H 6
(44.75%) 0.6689*Re 1 s(14.03%)p 1.39(19.47%)d 4.74(66.50%)
6. (0.85085) BD (1)Re 1- H 7
(44.75%) 0.6689*Re 1 s(14.03%)p 1.39(19.47%)d 4.74(66.50%)

***** Beta spin orbitals *****

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	0.58776	33.98054	2.91970	0.01199	36.91224
H 2	-0.05491	0.00000	0.55365	0.00126	0.55491
H 3	-0.00808	0.00000	0.50546	0.00261	0.50808
H 4	0.01321	0.00000	0.48613	0.00065	0.48679
H 5	0.01321	0.00000	0.48613	0.00065	0.48679
H 6	-0.02560	0.00000	0.52375	0.00185	0.52560
H 7	-0.02560	0.00000	0.52375	0.00185	0.52560
* Total *	0.50000	33.98054	5.99859	0.02087	40.00000

Total non-Lewis 0.36518 (0.913% of 40)

1. (0.95695) BD (1)Re 1- H 2
(45.08%) 0.6714*Re 1 s(19.40%)p 0.05(0.89%)d 4.11(79.70%)
2. (0.90414) BD (1)Re 1- H 3
(48.26%) 0.6947*Re 1 s(18.03%)p 0.04(0.65%)d 4.51(81.32%)
3. (0.97067) BD (1)Re 1- H 4
(51.82%) 0.7198*Re 1 s(20.23%)p 0.01(0.18%)d 3.94(79.60%)
4. (0.97067) BD (1)Re 1- H 5
(51.82%) 0.7198*Re 1 s(20.23%)p 0.01(0.18%)d 3.94(79.60%)
5. (0.92593) BD (1)Re 1- H 6

(47.16%) 0.6868*Re 1 s(11.03%)p 0.06(0.69%)d 8.00(88.28%)

6. (0.92593) BD (1)Re 1- H 7

(47.16%) 0.6868*Re 1 s(11.03%)p 0.06(0.69%)d 8.00(88.28%)

ReH₆ (Cs, narrow H'-Re-H')

Re 0.0000000123 0.0331640864 0.

H -0.0585067254 -1.2442529027 0.9909645

H 1.3785278421 -0.8815851702 0.

H -0.0585067254 -1.2442529027 -0.9909645

H -1.3876904877 0.0327658447 0.9307525

H 1.5138656583 0.8172528046 0.

H -1.3876904877 0.0327658447 -0.9307525

SCF Done: E(UB+HF-LYP) = -82.5493889862 A.U. after 10 cycles

Frequencies -- 398.6538 461.7164 634.7752

Frequencies -- 641.1063 650.0783 837.9041

Frequencies -- 947.9997 1007.6054 1151.5066

Frequencies -- 1847.0544 1955.0092 1955.9563

Frequencies -- 2006.2338 2119.8426 2143.0709

Natural Population

Natural					
Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	0.13135	67.96239	6.87841	0.02785	74.86865
H 2	0.07888	0.00000	0.91931	0.00181	0.92112
H 3	-0.00861	0.00000	1.00188	0.00673	1.00861
H 4	0.07888	0.00000	0.91931	0.00181	0.92112
H 5	-0.07340	0.00000	1.06856	0.00484	1.07340
H 6	-0.13371	0.00000	1.12943	0.00427	1.13371
H 7	-0.07340	0.00000	1.06856	0.00484	1.07340
* Total *	0.00000	67.96239	12.98546	0.05215	81.00000

Alpha spin orbitals

Natural Population

Natural					
Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	-0.44234	33.98234	3.94384	0.01616	37.94234
H 2	0.05347	0.00000	0.44565	0.00089	0.44653
H 3	-0.00807	0.00000	0.50384	0.00423	0.50807
H 4	0.05347	0.00000	0.44565	0.00089	0.44653
H 5	-0.03816	0.00000	0.53519	0.00297	0.53816

H 6	-0.08021	0.00000	0.57706	0.00315	0.58021
H 7	-0.03816	0.00000	0.53519	0.00297	0.53816
* Total *	-0.50000	33.98234	6.98641	0.03124	41.00000

Total non-Lewis 0.64216 (1.566% of 41)

1. (0.96144) BD (1)Re 1- H 2
(56.07%) 0.7488*Re 1 s(19.66%)p 0.02(0.36%)d 4.07(79.98%)
2. (0.82055) BD (1)Re 1- H 3
(46.20%) 0.6797*Re 1 s(15.26%)p 1.34(20.45%)d 4.21(64.29%)
3. (0.96144) BD (1)Re 1- H 4
(56.07%) 0.7488*Re 1 s(19.66%)p 0.02(0.36%)d 4.07(79.98%)
4. (0.87398) BD (1)Re 1- H 5
(45.58%) 0.6751*Re 1 s(14.78%)p 1.16(17.12%)d 4.61(68.09%)
5. (0.88658) BD (1)Re 1- H 6
(42.12%) 0.6490*Re 1 s(15.51%)p 1.20(18.61%)d 4.25(65.88%)
6. (0.87398) BD (1)Re 1- H 7
(45.58%) 0.6751*Re 1 s(14.78%)p 1.16(17.12%)d 4.61(68.09%)

***** Beta spin orbitals *****

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Re 1	0.57370	33.98004	2.93457	0.01170	36.92630
H 2	0.02541	0.00000	0.47366	0.00093	0.47459
H 3	-0.00053	0.00000	0.49803	0.00250	0.50053
H 4	0.02541	0.00000	0.47366	0.00093	0.47459
H 5	-0.03524	0.00000	0.53337	0.00187	0.53524
H 6	-0.05350	0.00000	0.55237	0.00112	0.55350
H 7	-0.03524	0.00000	0.53337	0.00187	0.53524
* Total *	0.50000	33.98004	5.99905	0.02091	40.00000

Total non-Lewis 0.37223 (0.931% of 40)

1. (0.96155) BD (1)Re 1- H 2
(53.02%) 0.7282*Re 1 s(19.79%)p 0.01(0.20%)d 4.04(80.01%)
2. (0.90414) BD (1)Re 1- H 3
(48.98%) 0.6999*Re 1 s(10.52%)p 0.06(0.64%)d 8.45(88.85%)
3. (0.96155) BD (1)Re 1- H 4
(53.02%) 0.7282*Re 1 s(19.79%)p 0.01(0.20%)d 4.04(80.01%)
4. (0.93487) BD (1)Re 1- H 5
(46.42%) 0.6813*Re 1 s(19.24%)p 0.04(0.77%)d 4.16(79.98%)
5. (0.95075) BD (1)Re 1- H 6

(45.08%) 0.6714*Re 1 s(11.36%)p 0.07(0.76%)d 7.74(87.88%)

6. (0.93487) BD (1)Re 1- H 7

(46.42%) 0.6813*Re 1 s(19.24%)p 0.04(0.77%)d 4.16(79.98%)

[WH,]⁻ (C3v eclipsed)

W 0. 0. -0.0050735303

H -1.135290777 0. 1.2930534538

H 0.5676453885 0.9831906536 1.2930534538

H 0.5676453885 -0.9831906536 1.2930534538

H -1.6263391345 0. -0.5828084428

H 0.8131695673 1.4084510057 -0.5828084428

H 0.8131695673 -1.4084510057 -0.5828084428

H 0. 0. -1.7552937877

SCF Done: E(RB+HF-LYP) = -71.9456809575 A.U. after 9 cycles

Frequencies --	457.2787	458.9486	654.8376
Frequencies --	702.5265	818.1596	818.5135
Frequencies --	844.9155	845.3785	1076.9450
Frequencies --	1079.0629	1144.2917	1757.2708
Frequencies --	1819.4613	1819.6172	1860.9708
Frequencies --	1868.5866	1868.6807	1935.8401

Natural Population

Atom No	Natural Charge	Core	Valence	Rydberg	Total
W 1	0.17283	67.96989	5.80203	0.05526	73.82717
H 2	-0.15757	0.00000	1.15330	0.00427	1.15757
H 3	-0.15757	0.00000	1.15330	0.00427	1.15757
H 4	-0.15757	0.00000	1.15330	0.00427	1.15757
H 5	-0.15976	0.00000	1.15797	0.00179	1.15976
H 6	-0.15976	0.00000	1.15797	0.00179	1.15976
H 7	-0.15976	0.00000	1.15797	0.00179	1.15976
H 8	-0.22085	0.00000	1.21492	0.00592	1.22085
* Total *	-1.00000	67.96989	13.95075	0.07936	82.00000

Total non-Lewis 1.03575 (1.263% of 82)

1. (1.82381) BD (1) W 1- H 2

(40.60%) 0.6372* W 1 s(12.05%)p 1.51(18.19%)d 5.79(69.76%)

2. (1.82381) BD (1) W 1- H 3

(40.60%) 0.6372* W 1 s(12.05%)p 1.51(18.19%)d 5.79(69.76%)

3. (1.82381) BD (1) W 1- H 4

- (40.60%) 0.6372* W 1 s(12.05%)p 1.51(18.19%)d 5.79(69.76%)
4. (1.93207) BD (1) W 1- H 5
(41.80%) 0.6466* W 1 s(16.97%)p 0.23(3.88%)d 4.66(79.14%)
5. (1.93207) BD (1) W 1- H 6
(41.80%) 0.6466* W 1 s(16.97%)p 0.23(3.88%)d 4.66(79.14%)
6. (1.93207) BD (1) W 1- H 7
(41.80%) 0.6466* W 1 s(16.97%)p 0.23(3.88%)d 4.66(79.14%)
7. (1.72678) BD (1) W 1- H 8
(34.88%) 0.5906* W 1 s(13.17%)p 2.65(34.97%)d 3.94(51.85%)

[WH,] (C3v staggered)

W 0. 0. -0.0307432011

H -1.0605138774 0. 1.3150340906

H 1.7190477941 0. 0.0680878065

H -0.8595238971 1.48873906 0.0680878065

H 0.5302569387 -0.9184319589 1.3150340906

H 0.5302569387 0.9184319589 1.3150340906

H -0.8595238971 -1.48873906 0.0680878065

H 0. 0. -1.8743688096

SCF Done: E(RB+HF-LYP) = -71.9405190873 A.U. after 9 cycles

Frequencies -- 335.0432 335.8216 698.6628

Frequencies -- 700.4109 701.6807 771.0017

Frequencies -- 888.6608 892.5588 1052.5802

Frequencies -- 1135.8689 1136.8105 1570.6932

Frequencies -- 1871.6539 1871.9646 1872.2775

Frequencies -- 1904.3568 1905.3054 1945.8503

Natural Population

Natural					
Atom No	Charge	Core	Valence	Rydberg	Total
W 1	0.22602	67.97245	5.73733	0.06421	73.77398
H 2	-0.10623	0.00000	1.10091	0.00532	1.10623
H 3	-0.16460	0.00000	1.16252	0.00209	1.16460
H 4	-0.16460	0.00000	1.16252	0.00209	1.16460
H 5	-0.10623	0.00000	1.10091	0.00532	1.10623
H 6	-0.10623	0.00000	1.10091	0.00532	1.10623
H 7	-0.16460	0.00000	1.16252	0.00209	1.16460
H 8	-0.41351	0.00000	1.40856	0.00494	1.41351
* Total *	-1.00000	67.97245	13.93617	0.09138	82.00000

Total non-Lewis 1.07687 (1.313% of 82)

1. (1.75951) BD (1) W 1- H 2
(42.03%) 0.6483* W 1 s(6.75%)p 3.24(21.88%)d10.57(71.36%)
2. (1.94267) BD (1) W 1- H 3
(41.70%) 0.6458* W 1 s(17.34%)p 0.05(0.82%)d 4.72(81.83%)
3. (1.94267) BD (1) W 1- H 4
(41.70%) 0.6458* W 1 s(17.34%)p 0.05(0.82%)d 4.72(81.83%)
4. (1.75951) BD (1) W 1- H 5
(42.03%) 0.6483* W 1 s(6.75%)p 3.24(21.88%)d10.57(71.36%)
5. (1.75951) BD (1) W 1- H 6
(42.03%) 0.6483* W 1 s(6.75%)p 3.24(21.88%)d10.57(71.36%)
6. (1.94267) BD (1) W 1- H 7
(41.70%) 0.6458* W 1 s(17.34%)p 0.05(0.82%)d 4.72(81.83%)
7. (1.84418) BD (1) W 1- H 8
(27.55%) 0.5249* W 1 s(32.91%)p 0.93(30.56%)d 1.11(36.53%)

[PdH₈]⁻

Pd 0. 0. -0.0342087131

H 0. 0. 1.4876453145

H 0. 1.683258915 0.0429777445

H 0. -1.683258915 0.0429777445

SCF Done: E(RB+HF-LYP) = -128.525277264 A.U. after 10 cycles

Frequencies -- 336.0882 653.9758 712.6447

Frequencies -- 1444.9332 1714.6176 2125.1941

Natural Population

Atom No	Charge	Core	Valence	Rydberg	Total
Pd 1	-0.21117	35.98904	10.12574	0.09638	46.21117
H 2	0.02562	0.00000	0.97244	0.00194	0.97438
H 3	-0.40723	0.00000	1.40103	0.00620	1.40723
H 4	-0.40723	0.00000	1.40103	0.00620	1.40723
* Total *	-1.00000	35.98904	13.90025	0.11071	50.00000

Total non-Lewis 0.71982 (1.440% of 50)

1. (1.94152) BD (1)Pd 1- H 2
(52.00%) 0.7211*Pd 1 s(40.39%)p 0.02(0.83%)d 1.46(58.78%)
2. (1.95113) BD (1)Pd 1- H 3
(38.13%) 0.6175*Pd 1 s(50.11%)p 0.08(3.91%)d 0.92(45.98%)

[PtH₄]²⁺ (Basis Set lacking 6p orbitals- see [PtH₂]- for details)

Pt 0. 0. 0.

H 0. 0. 1.6886091579

H 1.6886091579 0. 0.

H -1.6886091579 0. 0.

H 0. 0. -1.6886091579

SCF Done: E(RB+HF-LYP) = -121.356428611 A.U. after 7 cycles

Frequencies -- 699.3325 699.3325 814.5445

Frequencies -- 856.2008 895.3243 1555.8730

Frequencies -- 1555.8730 1904.4266 1928.5823

Natural Population

Natural					
Atom No	Charge	Core	Valence	Rydberg	Total
Pt 1	-0.30542	67.99935	10.30395	0.00213	78.30542
H 2	-0.42365	0.00000	1.41814	0.00551	1.42365
H 3	-0.42365	0.00000	1.41814	0.00551	1.42365
H 4	-0.42365	0.00000	1.41814	0.00551	1.42365
H 5	-0.42365	0.00000	1.41814	0.00551	1.42365
* Total *	-2.00000	67.99935	15.97651	0.02415	84.00000

Total non-Lewis 1.22047 (1.453% of 84)

1. (1.97301) BD (1)Pt 1- H 2

(40.44%) 0.6359*Pt 1 s(45.15%)p 0.00(0.00%)d 1.21(54.85%)

2. (1.97301) BD (1)Pt 1- H 3

(40.44%) 0.6359*Pt 1 s(45.15%)p 0.00(0.00%)d 1.21(54.85%)

[WF₆] MullikenPA, NPA

W 0. 0. 0.

F 0. 0. 1.8661371877

F 0. 0. -1.8661371877

F 0. 1.8661371877 0.

F 0. -1.8661371877 0.

F 1.8661371877 0. 0.

F -1.8661371877 0. 0.

SCF Done: E(RB+HF-LYP) = -667.181718078 A.U. after 5 cycles

Frequencies -- 123.1173 123.1173 123.1178

Frequencies -- 232.0862 232.0863 232.0864

Frequencies -- 295.8228 295.8228 295.8228

Frequencies -- 647.5950 647.5950 715.0583

Frequencies -- 715.0584 715.0586 725.7370

Natural Population

		Natural	-----			
Atom No	Charge	Core	Valence	Rydberg	Total	
W 1	2.57308	67.99929	3.35651	0.07113	71.42692	
F 2	-0.42885	1.99998	7.42558	0.00328	9.42885	
F 3	-0.42885	1.99998	7.42558	0.00328	9.42885	
F 4	-0.42885	1.99998	7.42558	0.00328	9.42885	
F 5	-0.42885	1.99998	7.42558	0.00328	9.42885	
F 6	-0.42885	1.99998	7.42558	0.00328	9.42885	
F 7	-0.42885	1.99998	7.42558	0.00328	9.42885	
* Total *	0.00000	79.99917	47.91000	0.09082	128.00000	

Total non-Lewis 2.29245 (1.791% of 128)

1. (1.99905) BD (1) W 1- F 2

(11.10%) 0.3331* W 1 s(0.00%)p 1.00(0.73%)d99.99(99.27%)

2. (1.99905) BD (2) W 1- F 2

(11.10%) 0.3331* W 1 s(0.00%)p 1.00(0.74%)d99.99(99.26%)

3. (1.98882) BD (3) W 1- F 2

(12.41%) 0.3523* W 1 s(33.33%)p 0.00(0.01%)d 2.00(66.66%)

4. (1.99905) BD (1) W 1- F 4

(11.10%) 0.3331* W 1 s(0.00%)p 1.00(0.73%)d99.99(99.27%)

5. (1.98882) BD (2) W 1- F 4

(12.41%) 0.3523* W 1 s(33.33%)p 0.00(0.01%)d 2.00(66.66%)

6. (1.98882) BD (1) W 1- F 6

(12.41%) 0.3523* W 1 s(33.33%)p 0.00(0.01%)d 2.00(66.66%)