17 November 2014

First principles static and dynamic calculations for the transition metal hydride series MH_4L_3 (M= Fe, Ru and Os; L = NH_3, PH_3 and PF_3)

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-- Supporting Information –-

Full reference 23:

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Table S1: Characteristics of the transition states and rate constants.

M	L	Isomer *(a)*	Type *(b)*	ν *(cm^{-1})(b)*	T_c *(K)(c)*	κ_{Wigner} *(d)*	k_{TST} *(s^{-1}) (e)*	k' *(s^{-1}) (f)*
Fe	**NH_3**	**Non-class. perp**	T.S.	-379.0	87	1.10	2.33E+08	2.56E+08
		TS scrambling	T.S.	-316.2	72	1.07	8.44E+11	9.03E+11
Fe	**PH_3**	**Non-class. perp**	T.S.	-119.2	27	1.01	1.30E+12	1.31E+12
		Classical	T.S.	-171.5	39	1.02	2.01E+10	2.05E+10
Fe	**PF_3**	**TS rotation**	T.S.	-107.1	25	1.01	6.31E+12	6.36E+12
		Classical	T.S.	-186.0	43	1.02	4.14E+08	4.24E+08
Ru	**NH_3**	**Non-class. Perp**	T.S.	-205.0	47	1.03	6.35E+09	6.54E+09
Ru	**PH_3**	**Non-class. perp**	T.S.	-274.4	63	1.05	4.75E+11	5.00E+11
		TS scrambling	T.S.	-433.4	99	1.13	8.44E+11	9.55E+11
Ru	**PF_3**	**Non-class. perp**	T.S.	-169.1	39	1.02	2.00E+12	2.04E+12
		TS scrambling	T.S.	-200.4	46	1.03	7.35E+08	7.56E+08
Os	**NH_3**	**Non-class. perp**	T.S.	-49.0	11	1.00	1.51E+07	1.52E+07
Os	**PH_3**	**Non-class. perp**	T.S.	-309.6	71	1.07	3.57E+09	3.81E+09
		TS scrambling	T.S.	-324.4	74	1.07	1.30E+12	1.40E+12
Os	**PF_3**	**Non-class. perp**	T.S.	-293.9	67	1.06	8.44E+11	8.95E+11
		TS scrambling	T.S.	-520.8	119	1.19	8.44E+11	1.01E+12

(a) See Scheme 2 in the Text for schematic representation of the complexes.

(b) All structures listed in this Table are transition states with a single imaginary frequency ν (in cm^{-1}).

(c) Crossover temperature (in K, see Reference 34):

$$T_c = \frac{h\nu}{2\pi k_B}$$

(d) Calculated at T = 350 K according to the following eq. (see References 35 and 36):

$$\kappa_{Wigner} = 1 + \frac{1}{24}\left(\frac{h|\nu|}{k_B T}\right)^2$$

(e) Rate constants calculated according to the Eyring equation, with T = 350 K, activation free energies ($\Delta G^{\neq}$) calculated at the PBE/SDD/6-311G** level (see Table 1) and a transmission coefficient of 1:

$$k_{TST} = \frac{k_B T}{h} e^{-\frac{\Delta G^{\neq}}{RT}}$$

(f) "Wigner-corrected" rate constants, calculated as:

$$k' = \kappa_{Wigner} \cdot k_{TST}$$

h, k_B and R are the Planck constant, the Boltzmann constant and the ideal gas constant, respectively.

Table S2: Geometrical parameters of the optimized complexes.[(a)]

M	L	Isomer *(b)*	Type *(c)*	d1 *(Å)*	d2 *(Å)*	d3 *(Å)*	Δd *(Å)*	α °	ϕ °	$\Delta E_{rel}[\Delta G_{rel}]$ kcal/mol
					$[MH_4L_3]$					
Fe	**NH_3**	**Non-classical**	Min.	0.99	1.76	2.02	1.03	171.9	0.1	0.0
		Non-clas. perp	T.S.	0.88	2.23	2.23	1.35	161.9	90.2	6.0 [7.2]
		Classical	Min.	1.67	1.49	1.67	0.00	175.5	0.1	1.3 [1.8]
		TS exchange	T.S.	1.35	1.59	1.86	0.51	174.1	0.0	1.2 [1.5]
Fe	**PH_3**	**Non-classical**	Min.	0.90	1.89	1.98	1.08	156.8	0.2	0.0
		Non-clas. perp	T.S.	0.88	2.19	2.13	1.25	148.0	90.4	1.2 [1.2]
		Classical	T.S.	1.54	1.77	1.55	0.01	166.0	0.0	5.1 [4.1]
Fe	**PF_3**	**Non-classical**	Min.	0.88	1.86	2.04	1.16	146.8	0.4	0.0
		Non-clas. perp	Min.	0.88	2.14	2.15	1.27	140.2	90.5	0.4 [-1.1]
		TS rotation	T.S.	0.87	2.03	2.14	1.27	141.1	74.6	0.4 [0.1]
		Classical	T.S.	1.48	1.87	1.60	0.12	159.4	0.0	7.7 [6.8]
Ru	**NH_3**	**Non-classical**	→ *classical* [(d)]							
		Non-clas. perp	T.S.	0.95	2.32	2.30	1.35	163.1	92.8	5.4 [4.9]
		Classical	Min.	1.81	1.66	1.82	0.01	175.2	0.0	0.0
Ru	**PH_3**	**Non-classical**	Min.	0.90	2.10	2.10	1.20	161.7	0.0	0.0
		Non-clas. perp	T.S.	0.87	2.38	2.21	1.34	154.8	90.8	2.3 [1.9]
		Classical	Min.	1.74	1.83	1.79	0.05	168.5	0.0	3.0 [2.0]
		TS exchange	T.S.	1.39	1.92	1.94	0.55	166.4	0.0	3.3 [1.5]
Ru	**PF_3**	**Non-classical**	Min.	0.87	2.09	2.14	1.27	155.5	0.1	0.0
		Non-clas. perp	T.S.	0.85	2.37	2.30	1.45	145.7	90.5	1.7 [0.9]
		TS exchange	T.S.	1.54	1.90	1.89	0.35	163.9	9.6	7.2 [6.4]
		Classical	Min.	1.72	1.87	1.82	0.10	164.9	0.0	7.0 [5.6]
Os	**NH_3**	**Non-classical**	→ *classical* [(d)]							
		Non-clas. perp	T.S.	1.42	2.30	2.43	1.01	157.1	90.2	9.0 [9.1]
		Classical	Min.	1.89	1.71	1.89	0.00	175.7	0.0	0.0
Os	**PH_3**	**Non-classical**	Min.	1.02	2.09	2.13	1.11	165.2	0.0	1.9 [1.5]
		Non-clas. perp	T.S.	0.91	2.39	2.26	1.35	157.1	90.7	5.4 [5.3]
		Classical	Min.	1.83	1.86	1.86	0.03	169.4	0.0	0.0
		TS exchange	T.S.	1.10	2.06	2.11	1.01	165.8	0.0	2.0 [1.2]
Os	**PF_3**	**Non-classical**	Min.	0.92	2.12	2.15	1.23	160.7	0.0	0.0
		Non-clas. perp	T.S.	0.87	2.39	2.30	1.43	152.1	90.7	2.7 [1.5]
		Classical	Min	1.83	1.88	1.87	0.04	166.2	0.0	1.6 [1.0]
		TS exchange	T.S.	1.30	1.99	2.03	0.73	164.8	0.0	2.5 [1.5]

(a) Static calculations. Geometries are computed at the PBE/SDD/6-31G** level. *d1*, *d2* and *d3* stand for d*(H1-H2)*, d(H2-H3) and d(H3-H4), respectively. $\Delta d = d3 - d1$. Relative energies and Free energies at the PBE/SDD/6-311+G** are also given (see Table 1 for more details).

(b) See Scheme 2 for schematic representation of the complexes.

(c) Indicates whether the structure is a minimum ("Min.") or a transition state (T.S.).

(d) The optimization leads to the classical isomer.

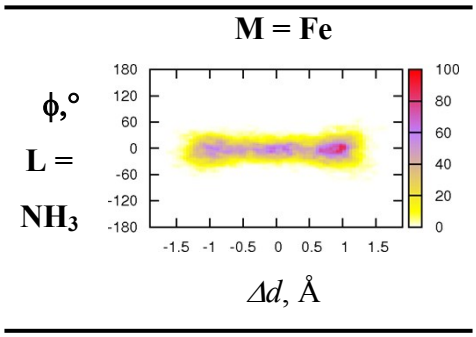

Figure S1: Correlation between the non-classical/classical hydride exchange and the rotational motion of H_2 in $[FeH_4(NH_3)_3]$ over 30 ps of MD, using a tighter criterion for convergence of the energy (10^{-7} h instead of 10^{-6} h) and a halved timestep (0.275 fs).

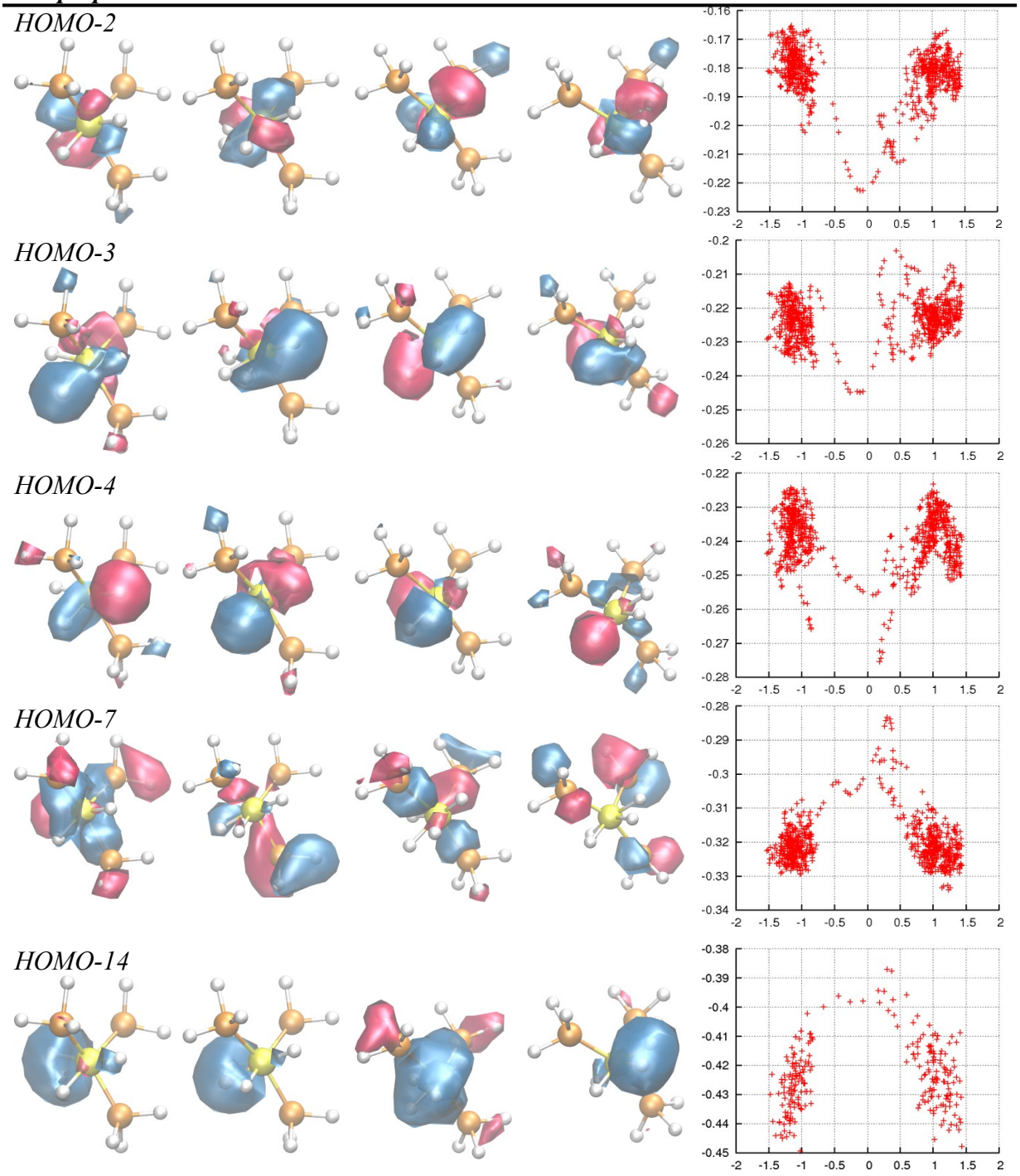

Figure S2: Time evolution of molecular orbitals during the scrambling process in $[FeH_4(PH_3)_3]$. The same isosurface value has been used to plot the orbitals and the complexes are shown in the same orientation.

Cartesian coordinates of selected complexes (PBE/SDD/6-31G** optimized geometries):

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17
[FeH4(NH3)3] – Classical (Minimum)
Fe     0.003474    -0.020037     0.000081
 N    -0.006295     0.022457     2.029552
 N     0.148809     0.022448    -2.024355
 N    -1.736510    -1.159644    -0.066458
 H     0.041088     0.999265     2.331067
 H    -0.813685    -0.398587     2.507811
 H     0.830545    -0.455793     2.373143
 H    -2.351340    -0.954872     0.728265
 H    -2.293017    -0.947906    -0.901262
 H    -1.536604    -2.162118    -0.063270
 H    -0.615488    -0.406234    -2.562780
 H     0.211003     0.999373    -2.322797
 H     1.013705    -0.448875    -2.301606
 H     1.494603     0.094412     0.057387
 H     0.763226    -1.410078     0.028877
 H     0.659788     1.324667     0.024841
 H    -1.004801     1.200516    -0.038152

17
[FeH4(NH3)3] – Non-classical (Minimum)
Fe    -0.003490    -0.291947     0.026835
 N    -2.031180    -0.403152    -0.017829
 N     2.018877    -0.390087    -0.126704
 N    -0.009573     1.806461     0.000585
 H    -2.400513    -1.000491     0.727400
 H    -2.577705     0.469403    -0.005821
 H    -2.222078    -0.870774    -0.907711
 H    -0.802748     2.226893     0.496936
 H     0.829641     2.229049     0.412780
 H    -0.059195     2.106984    -0.976833
 H     2.555365     0.487809    -0.170460
 H     2.162829    -0.879237    -1.013851
 H     2.438124    -0.963288     0.611121
 H    -0.008802    -1.787195    -0.322646
 H    -0.045168    -0.181285    -1.550411
 H     0.034048    -1.144739     1.319375
 H     0.039613    -0.215801     1.645674

17
[FeH4(NH3)3] – TS-exchange  (TS)
Fe     0.000007    -0.294921    -0.014224
 N     2.028163    -0.382414     0.041616
 N    -2.028166    -0.382444     0.041612
 N    -0.000024     1.792755    -0.011830
 H     2.381881    -0.959778    -0.726111
 H     2.549551     0.504206     0.016236
 H     2.268239    -0.848770     0.919976
 H     0.816591     2.184757    -0.492514
 H    -0.816181     2.184715    -0.493317
 H    -0.000473     2.144695     0.948263
 H    -2.549542     0.504187     0.016476
 H    -2.268231    -0.849014     0.919861
 H    -2.381906    -0.959609    -0.726253
 H     0.000071    -1.705499     0.530541
 H    -0.000043    -0.165566     1.570167
 H     0.000086    -1.392730    -1.027191
 H    -0.000024    -0.168932    -1.586103

17
[FeH4(NH3)3] – Non-classical perp. (TS)
Fe     0.000751    -0.281717     0.094265
 H     0.000978    -1.830909     0.107113
 H     0.810813     2.166165    -0.534959
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 H     0.000646    -0.270765    -1.485734
 H    -0.438100    -0.296233     1.662940
 H     0.439900    -0.295994     1.662863
 H    -0.006698     2.328081     0.886120
 H    -0.818502     2.161262    -0.537738
 H    -2.031328    -0.984246    -1.051093
 H     2.034558    -0.977838    -1.052458
 H    -2.457796    -1.013950     0.542876
 H     2.460021    -1.010719     0.541713
 H     2.577659     0.404866    -0.311475
 H    -2.577457     0.399278    -0.313937
 N    -0.003734     1.826846    -0.008279
 N     2.008656    -0.443771    -0.179260
 N    -2.006952    -0.447981    -0.179194

17
[FeH4(PH3)3] - Non-classical (Minimum)
Fe     0.003442    -0.348777     0.124655
 H    -0.005414    -1.818772    -0.255561
 H     0.026677     2.618361     1.379142
 H    -0.037029    -0.200441    -1.388782
 H     0.039715    -1.140140     1.503896
 H     0.046782    -0.275370     1.734465
 H    -1.069998     2.556642    -0.431834
 H     1.052391     2.557723    -0.472988
 H     2.490258    -1.501029    -1.319599
 H    -2.554632    -1.509339    -1.181512
 H    -2.952252    -1.191006     0.884903
 H     2.994799    -1.193777     0.725411
 H     2.961420     0.452171    -0.621941
 H    -2.990162     0.447532    -0.471672
 P     0.003834     1.826197     0.182617
 P     2.099909    -0.638992    -0.251278
 P    -2.109749    -0.640973    -0.139922

17
[FeH4(PH3)3] - Classical  (TS)
Fe     0.000000    -0.348521     0.003950
 P     2.138731    -0.611977    -0.000732
 P    -2.138731    -0.611977    -0.000732
 P     0.000000     1.825410     0.006878
 H     2.739918    -1.544986    -0.901926
 H     3.041773     0.468933    -0.291127
 H     2.822746    -1.059558     1.173118
 H     1.063345     2.545094    -0.631872
 H    -1.063344     2.545093    -0.631874
 H    -0.000002     2.606027     1.206466
 H    -3.041773     0.468932    -0.291129
 H    -2.822746    -1.059555     1.173119
 H    -2.739917    -1.544988    -0.901924
 H     0.000000    -1.594568     0.832437
 H     0.000000    -0.207980     1.519052
 H     0.000000    -1.507443    -0.934318
 H     0.000000    -0.075294    -1.503914

17
[FeH4(PH3)3] - Non-classical perp. (TS)
Fe    -0.000025    -0.264914     0.217001
 P    -2.056768    -0.716683    -0.163187
 P     2.056698    -0.716820    -0.163177
 P     0.000115     1.895843    -0.056523
 H    -2.942327    -1.198932     0.855856
 H    -2.973166     0.259919    -0.691982
 H    -2.358414    -1.732317    -1.118578
 H    -1.059051     2.541023    -0.782833
 H     0.000251     2.841016     1.026827
 H     1.059275     2.540871    -0.782975
 H     2.973076     0.259681    -0.692188
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 H     2.942313    -1.198912     0.855894
 H     2.358281    -1.732617    -1.118415
 H    -0.000132    -1.792042     0.310344
 H     0.000002    -0.399193    -1.297073
 H     0.439579    -0.218178     1.768214
 H    -0.439722    -0.217679     1.768177

17
[FeH4(PF3)3] - Non-classical (Minimum)
Fe     0.000337    -0.171024     0.154786
 P    -1.991737    -0.616935    -0.182888
 P     1.972448    -0.603406    -0.298413
 P    -0.004890     1.920289     0.220402
 F    -2.851429    -1.354570     0.954359
 F    -3.053921     0.521657    -0.575102
 F    -2.315818    -1.619890    -1.384628
 F    -1.190794     2.678528     0.993953
 F     1.221100     2.687492     0.918890
 F    -0.050304     2.764765    -1.137967
 F     2.999977     0.541976    -0.757259
 F     2.232655    -1.608660    -1.513703
 F     2.904289    -1.329596     0.788287
 H    -0.001847    -1.678709    -0.049591
 H    -0.043195    -0.108980    -1.350673
 H     0.046326    -0.844829     1.606184
 H     0.044847     0.020493     1.761807

17
[FeH4(PF3)3] - Non-classical perp. (Minimum)
Fe     0.023275    -0.274274     0.360109
 P    -1.912990    -0.922727     0.089802
 P     1.951887    -0.793522    -0.143393
 P    -0.065217     1.792949     0.036063
 F    -2.790602    -1.414059     1.338758
 F    -3.010771     0.019268    -0.605931
 F    -2.124710    -2.205028    -0.840547
 F    -0.171983     2.358193    -1.458387
 F    -1.264869     2.645407     0.683633
 F     1.142466     2.725996     0.542171
 F     2.893839     0.217256    -0.960460
 F     3.003181    -1.222177     0.989089
 F     2.135098    -2.061516    -1.099056
 H     0.088063    -1.780711     0.596808
 H    -0.059112    -0.501917    -1.128843
 H     0.548739    -0.124043     1.877782
 H    -0.324751    -0.152371     1.930487

17
[FeH4(PF3)3] - TS-rotation (TS)
Fe    -0.014459    -0.283937    -0.359584
 P     1.923196    -0.890462     0.010641
 P    -1.963543    -0.831377     0.011525
 P     0.043938     1.779454    -0.009411
 F     2.844507    -1.436637    -1.183068
 F     2.990471     0.096993     0.690880
 F     2.115314    -2.121893     1.011675
 F     0.138938     2.328666     1.491590
 F     1.233837     2.654392    -0.644709
 F    -1.174657     2.702211    -0.506894
 F    -2.952618     0.139836     0.821101
 F    -2.949541    -1.208847    -1.196186
 F    -2.195221    -2.141181     0.897573
 H    -0.058543    -1.790982    -0.594843
 H    -0.033258    -0.527206     1.128701
 H    -0.422620     0.032179    -1.890026
 H     0.377219    -0.317714    -1.923636

17
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[FeH4(PF3)3] - Classical (TS)
Fe    -0.002770    -0.221989     0.017374
 P    -2.049694    -0.583291    -0.004756
 P     2.040666    -0.603146     0.012218
 P     0.007635     1.860088    -0.054634
 F    -2.541050    -2.096184    -0.154677
 F    -2.943361    -0.181495     1.261001
 F    -2.965431     0.064583    -1.149130
 F    -1.201623     2.658261     0.631264
 F     1.218891     2.646519     0.641226
 F     0.017167     2.641949    -1.449509
 F     2.972031     0.035352    -1.124786
 F     2.518509    -2.120800    -0.133190
 F     2.927762    -0.209564     1.285160
 H    -0.005860    -1.514159    -0.736449
 H     0.004053    -0.098065    -1.487545
 H    -0.012342    -1.251949     1.112400
 H    -0.006902     0.176950     1.478391

17
[RuH4(NH3)3] - Classical (Minimum)
Ru    -0.002993    -0.333104     0.028016
 N    -2.147317    -0.429168     0.094828
 N     2.142456    -0.416405    -0.028251
 N    -0.013820     1.912677    -0.093838
 H    -2.427430    -0.963188     0.921411
 H    -2.647076     0.467869     0.134473
 H    -2.487070    -0.926778    -0.732081
 H    -0.824491     2.318369     0.383610
 H     0.810460     2.323071     0.355244
 H    -0.032186     2.215217    -1.069270
 H     2.638544     0.483409    -0.016749
 H     2.437052    -0.911883    -0.873550
 H     2.472439    -0.949096     0.780592
 H    -0.019624    -1.753870    -0.708011
 H    -0.051780    -0.206318    -1.657877
 H     0.027550    -1.642288     0.947931
 H     0.043330     0.010088     1.681963

17
[RuH4(NH3)3] - Non-classical perp. (TS)
Ru     0.004629    -0.246109     0.068748
 N    -2.120110    -0.415745    -0.211430
 N     2.137050    -0.367347    -0.210966
 N    -0.039238     2.063064    -0.011032
 H    -2.480514    -1.165495     0.382386
 H    -2.711000     0.412321    -0.062313
 H    -2.223040    -0.712569    -1.185181
 H     0.641677     2.404909    -0.696186
 H    -0.948893     2.417845    -0.326496
 H     0.163370     2.523484     0.880607
 H     2.711131     0.468711    -0.048974
 H     2.509004    -1.118900     0.373575
 H     2.247641    -0.650168    -1.188012
 H     0.030335    -1.860311     0.044263
 H     0.005366    -0.249204    -1.602147
 H     0.477078    -0.320322     1.718118
 H    -0.469734    -0.281322     1.719469

17
[RuH4(PH3)3] - Classical (Minimum)
Ru     0.054474     0.002149     0.002031
 P     0.141453     0.151402     2.278989
 P     0.314543     0.152323    -2.261630
 P    -1.864248    -1.331787    -0.071429
 H     0.400090     1.412901     2.894947
 H    -0.989285    -0.184570     3.095693
 H     1.097023    -0.595745     3.035069
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 H    -2.854172    -1.213674     0.955041
 H    -2.771541    -1.215441    -1.171825
 H    -1.811820    -2.758648    -0.068201
 H    -0.750716    -0.183604    -3.162091
 H     0.619007     1.414100    -2.855686
 H     1.325048    -0.594353    -2.943060
 H     1.667907     0.050474     0.063542
 H     0.811602    -1.466246     0.030614
 H     0.582807     1.523621     0.022497
 H    -1.163671     1.136090    -0.044156

17
[RuH4(PH3)3] - Non-classical (Minimum)
Ru     0.002351    -0.408290     0.082062
 P    -2.254401    -0.648032    -0.131518
 P     2.245177    -0.645702    -0.248679
 P     0.003352     1.919023     0.168022
 H    -3.083473    -1.156819     0.921030
 H    -3.099717     0.467480    -0.450572
 H    -2.755462    -1.510408    -1.151016
 H    -1.072238     2.647907    -0.439581
 H     0.033799     2.715494     1.360175
 H     1.045312     2.649007    -0.494393
 H     3.071842     0.470819    -0.610263
 H     3.128211    -1.154591     0.758968
 H     2.693350    -1.506815    -1.293550
 H    -0.008636    -1.972919    -0.373167
 H    -0.039897    -0.226326    -1.535560
 H     0.042215    -1.253608     1.595164
 H     0.048205    -0.386211     1.842877

17
[RuH4(PH3)3] - TS-exchange (TS)
Ru    -0.000005    -0.318540    -0.036376
 P     2.267036    -0.572336     0.056297
 P    -2.267049    -0.572308     0.056298
 P     0.000025     2.019067     0.008543
 H     2.929403    -1.425888    -0.878963
 H     3.171527     0.532670    -0.090657
 H     2.880546    -1.110592     1.227469
 H     1.062248     2.767512    -0.592951
 H    -1.062167     2.767544    -0.592968
 H     0.000025     2.733571     1.244698
 H    -3.171528     0.532708    -0.090658
 H    -2.880565    -1.110555     1.227471
 H    -2.929426    -1.425854    -0.878961
 H    -0.000002    -1.826844     0.558545
 H    -0.000005    -0.197143     1.614648
 H    -0.000013    -1.338509    -1.295473
 H    -0.000003     0.000769    -1.668757

17
[RuH4(PH3)3] - Non-classical perp.(TS)
Ru    -0.000019    -0.283946     0.158276
 P    -2.225763    -0.624485    -0.205026
 P     2.225724    -0.624593    -0.205014
 P     0.000091     2.026757    -0.046548
 H    -3.108558    -1.117832     0.806723
 H    -3.095413     0.425704    -0.655130
 H    -2.593591    -1.568249    -1.207137
 H    -1.056945     2.693545    -0.754263
 H     0.000089     2.953584     1.052849
 H     1.057224     2.693460    -0.754195
 H     3.095339     0.425539    -0.655325
 H     3.108578    -1.117758     0.806772
 H     2.593530    -1.568502    -1.206995
 H    -0.000078    -1.921127     0.157673
 H     0.000028    -0.416821    -1.457825
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 H     0.434341    -0.326546     1.875770
 H    -0.434502    -0.326558     1.875734

17
[OsH4(PH3)3] - Classical (Minimum)
Os     0.066642     0.012943     0.002474
 P     0.141725     0.150197     2.303360
 P     0.316895     0.150839    -2.285960
 P    -1.874204    -1.332313    -0.071741
 H     0.395054     1.410881     2.923295
 H    -0.994525    -0.193756     3.108717
 H     1.095882    -0.601717     3.056847
 H    -2.859632    -1.215339     0.958385
 H    -2.778563    -1.214711    -1.173650
 H    -1.802854    -2.756604    -0.069449
 H    -0.754495    -0.193252    -3.175728
 H     0.616342     1.411771    -2.884463
 H     1.326000    -0.600567    -2.964652
 H     1.715077     0.071109     0.065402
 H     0.789683    -1.507666     0.029827
 H     0.609088     1.567320     0.023398
 H    -1.199615     1.139860    -0.045716

17
[OsH4(PH3)3] - Non-classical (Minimum)
Os     0.001659    -0.431378     0.055425
 P    -2.287525    -0.642314    -0.094813
 P     2.280109    -0.639889    -0.213965
 P     0.002819     1.920513     0.145830
 H    -3.087879    -1.118807     0.992989
 H    -3.117431     0.485455    -0.408395
 H    -2.824890    -1.514445    -1.087407
 H    -1.075279     2.645729    -0.458992
 H     0.032736     2.693661     1.349857
 H     1.048429     2.646780    -0.512432
 H     3.091503     0.489022    -0.569157
 H     3.136412    -1.116639     0.830242
 H     2.765922    -1.510529    -1.234057
 H    -0.011519    -2.000957    -0.482093
 H    -0.041757    -0.190196    -1.601930
 H     0.039900    -1.348855     1.499976
 H     0.046783    -0.367139     1.788921

17
[OsH4(PH3)3] - TS-exchange (TS)
Os    -0.000042    -0.254801     0.054035
 P    -2.286910    -0.474023    -0.126769
 P     2.286764    -0.474393    -0.126773
 P     0.000319     2.101050    -0.004306
 H    -3.105700    -0.878678     0.975846
 H    -3.108469     0.632476    -0.525901
 H    -2.810000    -1.406801    -1.070770
 H    -1.060443     2.785602    -0.681483
 H    -0.002990     2.940261     1.153787
 H     1.065017     2.785621    -0.675358
 H     3.108869     0.633022    -0.522304
 H     2.809770    -1.404530    -1.073426
 H     3.105002    -0.882727     0.974881
 H    -0.000101    -1.838908    -0.431851
 H    -0.000192    -0.092852    -1.621201
 H     0.000071    -1.133920     1.499570
 H    -0.000243    -0.063215     1.759281

17
[OsH4(PH3)3] - Non-classical perp. (TS)
Os    -0.000016    -0.232881     0.111983
 P    -2.261194    -0.521643    -0.242893
 P     2.261165    -0.521759    -0.242879
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P	0.000101	2.096497	-0.047992
H	-3.138081	-1.028290	0.765210
H	-3.106727	0.563228	-0.652859
H	-2.642863	-1.428672	-1.272648
H	-1.059683	2.775372	-0.740641
H	0.000075	2.996387	1.073647
H	1.060007	2.775291	-0.740532
H	3.106652	0.563042	-0.653128
H	3.138128	-1.028159	0.765283
H	2.642807	-1.428992	-1.272464
H	-0.000078	-1.904180	0.112297
H	0.000036	-0.359162	-1.540799
H	0.452508	-0.296620	1.826196
H	-0.452683	-0.296692	1.826147