Supplementary Material (ESI) for Chemical Communications

Dihydrogen complexes: striking effect of ion pairing to BF_4^- on the rotation of coordinated dihydrogen and the ^{19}F relaxation time

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Electronic Supplementary Information

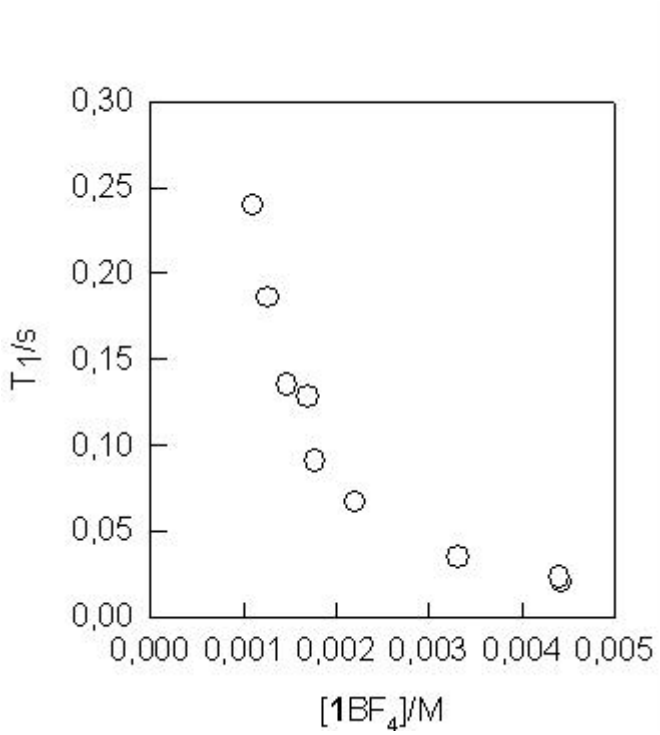

Figure S1. The effect of dilution on the T_1 values for the ^{19}F NMR signal at 25ºC in a solution of **1**BF_4 (4.4×10^{-3}M) in acetone-d_6.

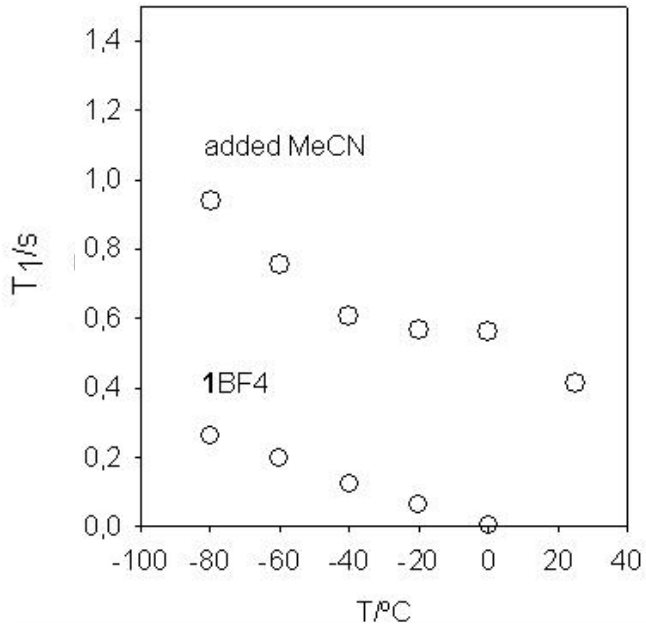

Figure S2. The effect of adding MeCN (0.1 ml) dilution on the T_1 values for the ^{19}F NMR signal at 25ºC for a solution of **1**BF_4 (0.5 ml, 7×10^{-3}M) in acetone-d_6.

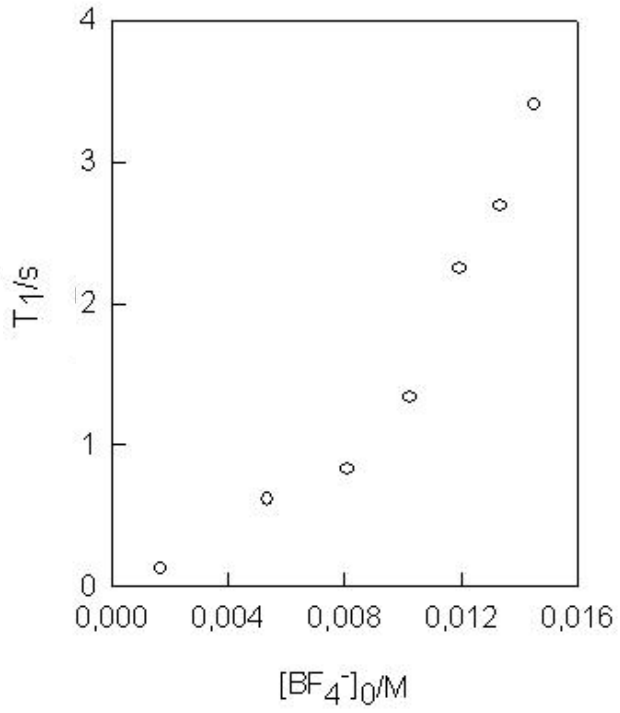

Figure S3. The effect of adding Bu_4NBF_4 on the T_1 values for the ^{19}F NMR signal at 25ºC for a solution of **1**BF_4 (1.7×10^{-3}M) in acetone-d_6.

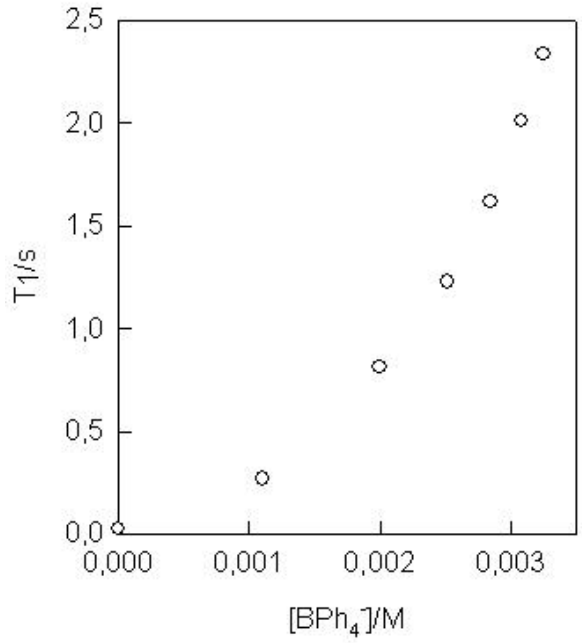

Figure S4. The effect of adding Bu_4NBPh_4 on the T_1 values for the ^{19}F NMR signal at 25ºC for a solution of **1**BF_4 (1.5×10^{-3}M) in acetone-d_6.

Computational details

All calculations were carried out with the Gaussian 03 package.[1] During the optimization procedure, QM/MM calculations were performed using the two-layered ONIOM method.[2-4] Phenyl groups on PPh_3 ligands were treated at the Universal Force Field (UFF) level,[5] while the rest of the complex or the ion-pair, including the counteranion BF_4^-, was calculated at the B3LYP and M05-2X levels.[6] The results obtained with both functional were similar, and so only those obtained with M05-2X are detailed, although for comparison the energies derived with B3LYP are also included below in the Table of absolute energies. The basis set for the Ru and Fe atoms was that associated with the pseudopotential,[7, 8] with a standard double-zeta LanL2DZ contraction,[1] supplemented in the case of Ru with a set of f-polarization fuctions.[9] The remaining atoms (P, B, F, C and H) were represented with 6-31G(d,p) basis set.[10] The nature of each stationary point was checked by diagonalizing the Hessian matrix to determine the number of imaginary frequencies (zero for the local minima and one for the transition states). Especially, the lone imaginary frequency of each TS displayed the desired displacement orientation, and its validity was further examined by intrinsic reaction coordinate (IRC) calculations.[11]

All the energies employed in the manuscript have been obtained by single-point DFT (M05-2X) calculations on the QM/MM optimized structures. They have been obtained adding up the solvation free energy in dichloromethane to the potential energy in the gas phase. In order to determine this magnitude, solvent effects were taken into account by means of the CPCM approach,[12, 13] and individual solvation cavities were added on the H atoms of the dihydrogen ligands. The dielectric constant was set to ε=8.93 to simulate dichloromethane (CH_2Cl_2) as the solvent medium and the same ECP and basis sets were used for the atoms of the previous QM layer, while the 6-31G(d,p) basis set was used to represent C and H atoms of the phenyl groups.

References

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Absolute energies (Hartrees)

All values were obtained at the M05-2X level, except those in the last column that were obtained with B3LYP.

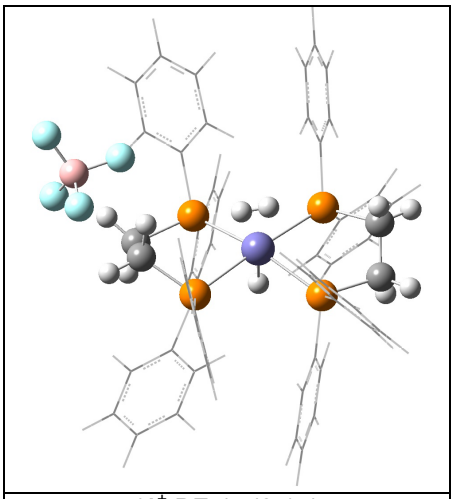
QM/MM calculations

	TS imaginary frecuencies (cm^{-1})	E(QM/MM, gas phase)	E(QM, CH_2Cl_2)	ΔE(QM, CH_2Cl_2, kcal)	ΔE(QM, CH_2Cl_2, kcal) (B3LYP)
1$^+$		-1652.00875529044	-3500.6629824		
TS for rotation of coordinated H_2 in **1**$^+$	-580.1	-1652.00677649101	-3500.6619091	0.67	0.53
(**1**$^+$,BF_4^-)		-2076.6478831141	-3925.2458253		
TS for rotation of coordinated H_2 in the (**1**$^+$,BF_4^-) ion pair	-390.6	-2076.6427200900	-3925.241839	2.5	1.87
(**1**$^+$,BF_4^-)$_b$		-2076.61936205590	-3925.2208139	2.69	2.14
(**1**$^+$,BF_4^-)$_c$		-2076.63784574674	-3925.2415411	15.69	7.17
2$^+$		-974.370228258624	-2360.824662		
TS for rotation of coordinated H_2 in **2**$^+$	-313.9	-974.365588831141	-2360.819303	3.36	2.50
(**2**$^+$,BF_4^-)		-1398.98922331922	-2785.413147		
TS for rotation of coordinated H_2 in the (**2**$^+$,BF_4^-) ion pair	-400.8	-1398.98247163709	-2785.399838	8.35	8.47
(**2**$^+$,BF_4^-)$_b$		-1398.9833462281	-2785.41202	0.71	0.67
(**2**$^+$,BF_4^-)$_c$		-1398.9483691722	-2785.392888	12.71	11.93

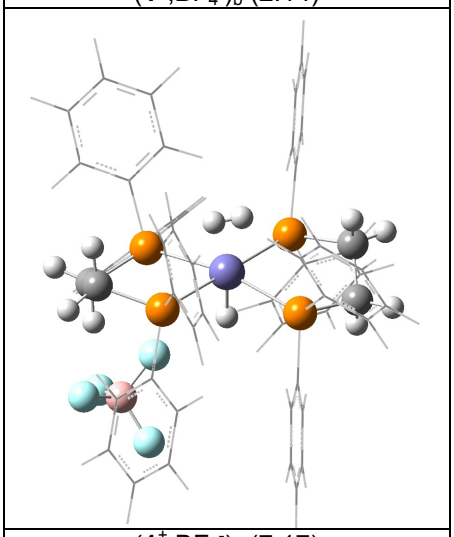
QM calculations on the simplified model (Ph groups replaced by H atoms)

	TS imaginary frecuencies (cm^{-1})	E(QM,gas phase)	E(QM,CH_2Cl_2)	ΔE(QM, CH_2Cl_2, kcal)	ΔE(QM, CH_2Cl_2, kcal) (B3LYP)
BF_4^-		-424.4825818	-424.5734231		
1s$^+$		-1652.2527640	-1652.31457		
TS for rotation of coordinated H_2 in **1s**$^+$	-416.0	-1652.252254	-1652.31399	0.36	0.28
(**1s**$^+$,BF_4^-)		-2076.8760998	-2076.9084		
TS for rotation of coordinated H_2 in the (**1s**$^+$,BF_4^-) ion pair	-216.3	-2076.872610	-2076.905655	1.72	1.75
2s$^+$		-974.5173224	-974.6105238	2.51	2.92
TS for rotation of coordinated H_2 in **2s**$^+$	-192.1	-974.5135914	-974.6065253		
(**2s**$^+$,BF_4^-)		-1399.1761447	-1399.205417	3.25	3.23
TS for rotation of coordinated H_2 in the (**2s**$^+$,BF_4^-) ion pair	-548.9	-1399.1709144	-1399.200239		

Optimized geometries for the ion pairs with the anion approaching to the metal complexes at different sites. The values in parentheses correspond to the relative energy (kcal) at the M05-2X level with respect to the most stable ion pair, i.e. that with BF_4^- approaching to H_2.



($\mathbf{1}^+$,BF_4^-)$_b$ (2.14)



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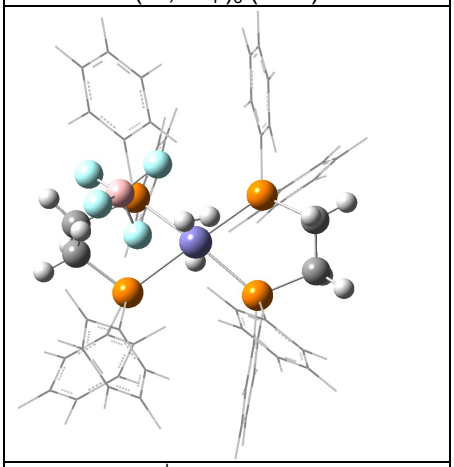
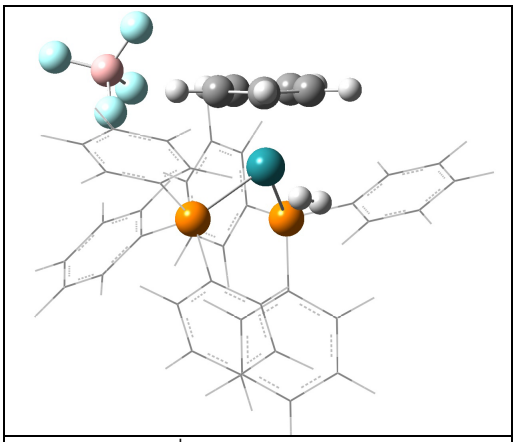
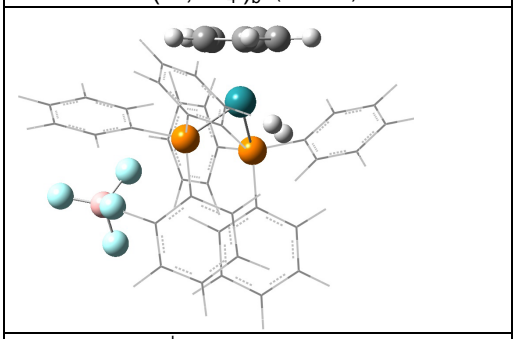


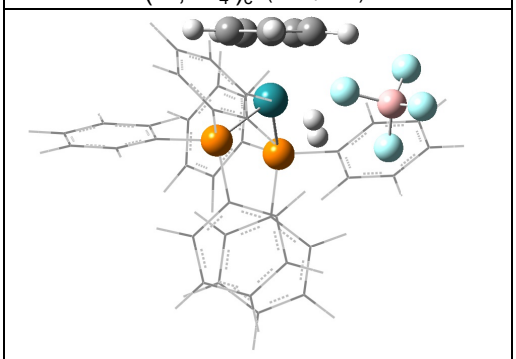
($\mathbf{1}^+$,BF_4^-) (0.00)



$(\mathbf{2}^{+},BF_4^{-})_b$ (0.71)



$(\mathbf{2}^{+},BF_4^{-})_c$ (12.71)

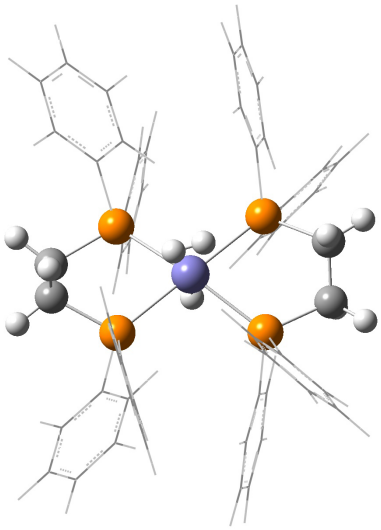


$(\mathbf{2}^{+},BF_4^{-})$ (0.00)

Cartesian coordinates

QM/MM calculations

1^+



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C	-3.597383	-3.499540	-1.976485
C	-4.473809	-3.280451	-2.974753
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C	3.535706	-3.884103	-1.747924

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H	-1.343794	-0.439872	4.295402
H	1.347343	-0.444312	-4.300982
H	0.405386	-1.677051	-3.464569
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H	-0.263085	1.309097	-3.565376

TS for rotation of coordinated H_2 in 1^+

C	-3.730281	-0.873144	-3.305292
C	-2.810349	-1.180352	-2.288622
C	-2.903827	-2.437909	-1.678483
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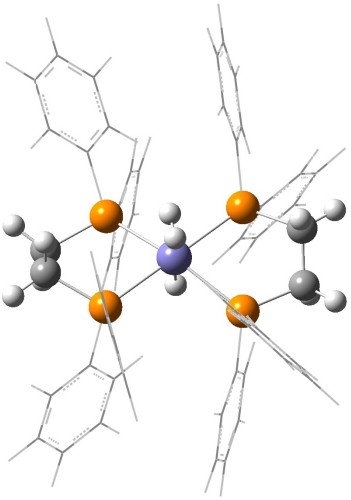

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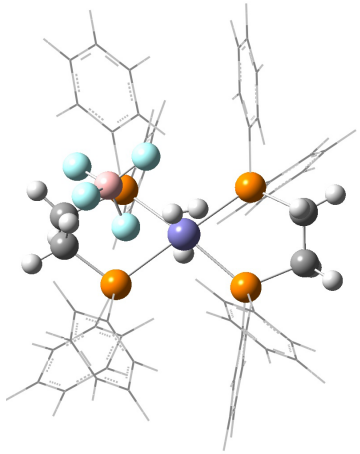
C	2.896482	-2.427282	1.640604
C	-2.799197	-1.633740	1.710954
C	-2.471180	-2.988804	1.892398
C	-3.464765	-3.966979	1.748629
C	-4.721570	-3.610298	1.427259
C	-5.039968	-2.316242	1.234413
C	-4.066382	-1.313119	1.370923
C	0.600558	-0.670990	-3.456081
C	-0.632977	0.254841	-3.464556
C	2.797971	-1.602894	-1.751308
C	4.118052	-1.277829	-1.400073
C	5.074091	-2.290439	-1.279550
C	4.711538	-3.625098	-1.495379
C	3.446211	-3.947009	-1.811731
C	2.465875	-2.953968	-1.939489
H	-0.387431	-2.020585	-0.095653
H	0.369715	-2.029226	0.038051
H	0.003773	1.134745	0.011254
H	2.214004	-2.698189	0.858846
H	3.952489	-4.301026	1.489654
H	5.531834	-3.783067	3.249027
H	5.415812	-1.665299	4.422086
H	3.684509	-0.004092	3.823859
H	4.411119	-0.255746	-1.210550
H	6.092610	-2.043151	-1.009835

H	5.456050	-4.404465	-1.394831
H	3.177553	-4.984970	-1.961202
H	1.449464	-3.246211	-2.165190
H	-2.218421	-2.741995	-0.911154
H	-3.982904	-4.298186	-1.591967
H	-5.556156	-3.701414	-3.324852
H	-5.430035	-1.558294	-4.434063
H	-3.694727	0.082013	-3.813361
H	-4.327694	0.621440	-1.005158
H	-4.418616	4.859340	-1.005176
H	-5.528891	2.740461	-0.668415
H	-2.098005	4.955945	-1.669794
H	-0.801369	2.893280	-2.020810
H	-3.554276	0.163446	3.876459
H	-1.384861	2.482650	0.960868
H	-2.602110	4.491274	1.682166
H	-4.291920	4.324059	3.493718
H	-4.731710	2.140402	4.575162
H	4.272394	0.578902	1.011787
H	5.512770	2.676723	0.710186
H	4.398876	4.856975	1.109547
H	2.070469	4.923922	1.785415
H	0.802587	2.836644	2.079699
H	-1.458757	-3.291781	2.121231
H	-3.216925	-5.011458	1.888067
H	-5.482346	-4.372195	1.312953
H	-4.352523	-0.287617	1.189608
H	-6.052602	-2.045653	0.963676
H	3.565592	0.236000	-3.876109
H	4.769707	2.283689	-4.530578
H	4.298143	4.429630	-3.382280
H	2.597512	4.521375	-1.582302
H	1.390856	2.495405	-0.920167
H	1.284652	-0.051247	4.302106
H	0.313387	1.218595	3.585201
H	-0.268722	-1.781576	3.407041
H	-1.222730	-0.607369	4.313368
H	1.227660	-0.516156	-4.331806
H	0.275698	-1.712386	-3.452844
H	-1.283680	0.033855	-4.307555
H	-0.312415	1.290802	-3.566112

(1^+,BF_4^-)

C	3.297799	-2.360523	2.644983
C	2.520569	-1.981226	1.538877
C	2.718346	-2.654870	0.332168
C	3.674308	-3.676399	0.252515
C	4.410786	-4.011768	1.328552
C	4.245654	-3.383695	2.508301
P	1.272457	-0.654478	1.681525
C	2.241250	0.737501	2.368665
C	3.628974	0.842155	2.176919
C	4.319468	1.948633	2.689130
C	3.665255	2.918578	3.355251
C	2.333523	2.858411	3.543090
C	1.590991	1.776369	3.052035
Fe	0.057513	0.055892	-0.207196
P	-1.813017	-0.696700	1.282702
C	-2.564220	0.479588	2.478457
C	-3.462868	0.034917	3.466421

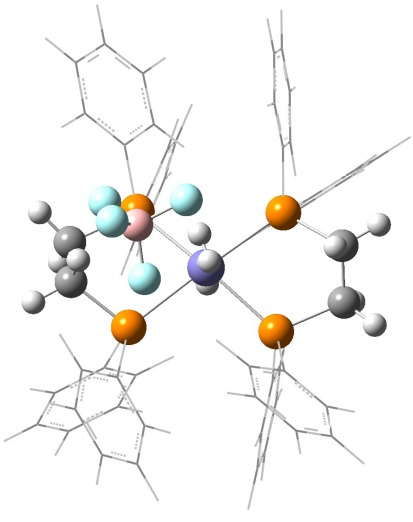


C	-4.039392	0.943240	4.359216
C	-3.726651	2.301642	4.275234
C	-2.836343	2.751889	3.298676
C	-2.258739	1.844854	2.406405
P	-1.167952	1.307271	-1.824640
C	-2.087166	2.716900	-1.096813
C	-3.437717	2.765617	-1.070627
C	-4.099316	3.844614	-0.468731
C	-3.361380	4.884397	0.107668
C	-2.020795	4.850744	0.080120
C	-1.357100	3.773666	-0.520890
P	1.828891	0.815048	-1.669703
C	2.732103	2.367983	-1.303342
C	2.433063	3.126297	-0.164027
C	3.130585	4.309027	0.089985
C	4.122783	4.727509	-0.798666
C	4.406026	3.963405	-1.936334
C	3.733444	2.825965	-2.183289
C	-0.095075	2.125198	-3.128743
C	1.127435	1.218544	-3.354093
C	-2.409953	0.414088	-2.830031
C	-3.122374	1.070999	-3.850962
C	-4.069389	0.359392	-4.600377
C	-4.290058	-0.943529	-4.345866
C	-3.607007	-1.578403	-3.374260
C	-2.651037	-0.891139	-2.608656
C	3.184655	-0.364788	-2.022776
C	2.981861	-1.426269	-2.923808
C	4.024607	-2.327670	-3.177767
C	5.208409	-2.183502	-2.555139
C	5.405733	-1.180219	-1.679111
C	4.381026	-0.259870	-1.404386
C	-1.032288	-1.885005	2.502780
C	0.222220	-1.240445	3.106848
C	-3.385575	-1.518705	0.812594
C	-4.370127	-0.765733	0.161614
C	-5.570899	-1.365031	-0.226316
C	-5.796365	-2.717852	0.049591
C	-4.870144	-3.446596	0.693894
C	-3.656464	-2.871421	1.094606
F	-1.180817	-5.418034	-0.197034
B	-0.342195	-4.325455	-0.174584
F	-1.134969	-3.117493	-0.246351
F	0.362083	-4.251053	1.049077
F	0.539029	-4.304176	-1.248683
H	-0.101903	-1.696247	-0.822507
H	0.232810	-1.240782	-1.357277
H	0.068142	1.351630	0.515958
H	-2.129092	-1.420898	-1.831680
H	-3.797741	-2.625740	-3.176874
H	-5.025342	-1.486299	-4.926529
H	-4.626248	0.861093	-5.381455
H	-2.966458	2.123032	-4.050050
H	-4.209649	0.280913	-0.034129
H	-6.326246	-0.782112	-0.737194
H	-6.728194	-3.177793	-0.253813
H	-5.061791	-4.490685	0.906636
H	-2.943206	-3.494808	1.611391
H	2.128600	-2.409341	-0.532531
H	3.819226	-4.200663	-0.683333
H	5.146411	-4.801877	1.244480

H	4.848840	-3.670930	3.360123
H	3.183069	-1.862610	3.599176
H	4.179122	0.090693	1.630389
H	4.218518	3.766919	3.738193
H	5.388945	2.026136	2.540291
H	1.828007	3.657601	4.070051
H	0.519409	1.766365	3.189731
H	3.980980	2.254974	-3.068918
H	1.668089	2.818840	0.523190
H	2.903544	4.896889	0.969921
H	4.669981	5.641776	-0.608922
H	5.175506	4.292844	-2.622918
H	-4.039705	1.982790	-1.502404
H	-5.181090	3.872387	-0.446875
H	-3.873664	5.715301	0.575557
H	-1.449270	5.654061	0.527220
H	-0.278070	3.760949	-0.523636
H	2.027829	-1.575089	-3.408730
H	3.872598	-3.146190	-3.869668
H	6.007175	-2.887074	-2.753213
H	4.570620	0.527274	-0.688897
H	6.360331	-1.083360	-1.177837
H	-3.730515	-1.010255	3.541747
H	-4.732000	0.593884	5.113961
H	-4.174421	3.004668	4.965565
H	-2.592861	3.804479	3.231951
H	-1.572712	2.214504	1.668401
H	-0.622654	2.302647	-4.062617
H	0.229298	3.095622	-2.751158
H	0.791499	0.284036	-3.806312
H	1.852939	1.675112	-4.024225
H	-1.718166	-2.190774	3.290714
H	-0.737172	-2.762212	1.927858
H	0.753931	-1.966083	3.718003
H	-0.039811	-0.396591	3.744352

TS for rotation of coordinated H_2 in the (1^+,BF_4^-) ion pair

C	3.474632	-1.932447	2.927782
C	2.723614	-1.742212	1.755635
C	3.079375	-2.479763	0.623440
C	4.152771	-3.378673	0.683274
C	4.855496	-3.533277	1.820765
C	4.544268	-2.837607	2.930426
P	1.324966	-0.559261	1.737548
C	2.132307	0.962356	2.357790
C	3.494218	1.217781	2.122449
C	4.065502	2.414422	2.575221
C	3.318763	3.331552	3.218250
C	2.006307	3.130022	3.439953
C	1.382145	1.950684	3.012365
Fe	0.052281	-0.026670	-0.095872
P	-1.783258	-0.724744	1.342349
C	-2.517012	0.493281	2.506415
C	-3.340352	0.077349	3.569532
C	-3.909776	1.017768	4.433229
C	-3.668820	2.379985	4.242070
C	-2.860145	2.802270	3.185286
C	-2.290055	1.863155	2.321902
P	-1.255941	1.088752	-1.880409
C	-2.145347	2.549467	-1.216597

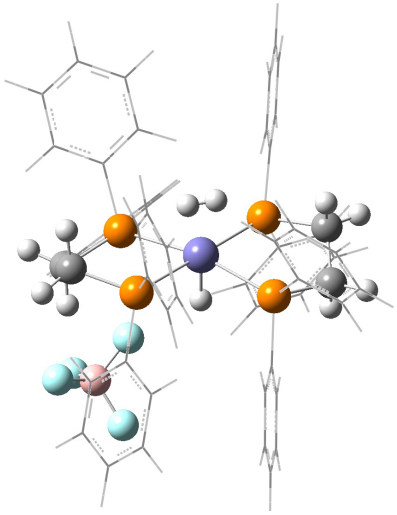


C	-3.492983	2.589647	-1.116334
C	-4.132976	3.706686	-0.562575
C	-3.376557	4.793123	-0.109658
C	-2.039261	4.767181	-0.209382
C	-1.397302	3.652209	-0.763050
P	1.761550	0.673637	-1.754705
C	2.605781	2.285983	-1.526802
C	2.328180	3.096738	-0.418296
C	2.976807	4.324549	-0.271516
C	3.902512	4.733366	-1.233268
C	4.170214	3.913213	-2.335075
C	3.543815	2.732551	-2.479484
C	-0.224642	1.813459	-3.274116
C	1.009572	0.913010	-3.445720
C	-2.551236	0.164421	-2.791896
C	-3.279325	0.781676	-3.827396
C	-4.270774	0.057624	-4.503672
C	-4.522896	-1.219535	-4.163901
C	-3.830318	-1.815752	-3.175116
C	-2.829987	-1.115062	-2.481640
C	3.158566	-0.469569	-2.056186
C	2.976365	-1.610939	-2.858148
C	4.053156	-2.480494	-3.079128
C	5.250631	-2.228130	-2.520233
C	5.428942	-1.147521	-1.736894
C	4.369219	-0.258192	-1.494515
C	-0.953073	-1.859458	2.576798
C	0.284719	-1.170162	3.167307
C	-3.359427	-1.585867	0.964669
C	-4.397388	-0.861719	0.364140
C	-5.603825	-1.492429	0.050679
C	-5.781061	-2.847400	0.349911
C	-4.802518	-3.548495	0.945613
C	-3.581929	-2.941695	1.271859
F	-0.388933	-5.518430	-0.291869
B	-0.079470	-4.176326	-0.284359
F	-1.258729	-3.387788	-0.322507
F	0.602198	-3.831464	0.919923
F	0.724997	-3.819080	-1.376137
H	-0.211153	-1.521517	-1.073644
H	0.465664	-1.642153	-0.729342
H	0.023997	1.321389	0.429013
H	-2.310253	-1.612701	-1.685011
H	-4.048917	-2.841550	-2.906245
H	-5.292881	-1.771935	-4.687738
H	-4.837368	0.529808	-5.296080
H	-3.102330	1.815590	-4.092616
H	-4.274977	0.187515	0.152142
H	-6.400923	-0.932030	-0.420385
H	-6.717521	-3.331641	0.104031
H	-4.956750	-4.594923	1.176504
H	-2.824313	-3.544580	1.748618
H	2.526399	-2.382198	-0.290163
H	4.417275	-3.954127	-0.194541
H	5.683622	-4.230547	1.844122
H	5.123688	-2.978048	3.834047
H	3.243815	-1.378175	3.828526
H	4.111859	0.514760	1.582135
H	3.779584	4.252275	3.553443
H	5.115475	2.606619	2.394830
H	1.423811	3.888684	3.947052

H	0.324168	1.825313	3.181623
H	3.780288	2.118491	-3.338723
H	1.617456	2.795014	0.327946
H	2.764024	4.954067	0.582785
H	4.411891	5.682282	-1.126496
H	4.890486	4.233917	-3.076951
H	-4.108538	1.770255	-1.450419
H	-5.212072	3.727470	-0.481405
H	-3.871866	5.653599	0.321613
H	-1.453252	5.606582	0.142575
H	-0.321004	3.648235	-0.825498
H	2.013914	-1.842672	-3.291542
H	3.917597	-3.360092	-3.695358
H	6.076385	-2.906792	-2.693057
H	4.542920	0.588941	-0.845885
H	6.394787	-0.965090	-1.283267
H	-3.558355	-0.970338	3.724594
H	-4.542908	0.690147	5.247604
H	-4.111268	3.107652	4.909935
H	-2.674859	3.857857	3.033425
H	-1.668925	2.211227	1.518365
H	-0.772686	1.893222	-4.209505
H	0.086381	2.820683	-2.995974
H	0.681906	-0.066902	-3.796737
H	1.707045	1.316623	-4.176720
H	-1.619717	-2.183712	3.373592
H	-0.632517	-2.727400	1.999545
H	0.839616	-1.882906	3.773222
H	0.000426	-0.340823	3.813062

$(\mathbf{1}^{+},BF_4^{-})_c$

C	-3.494494	-3.232874	-2.083855
C	-2.608504	-2.719062	-1.122029
C	-2.574676	-3.334895	0.134809
C	-3.422041	-4.418161	0.403401
C	-4.266782	-4.879077	-0.537770
C	-4.319985	-4.317851	-1.760251
P	-1.513313	-1.299637	-1.519013
C	-2.672644	-0.084548	-2.240612
C	-4.033079	-0.064572	-1.891637
C	-4.891707	0.862914	-2.496348
C	-4.424791	1.741529	-3.403349
C	-3.123106	1.762980	-3.747153
C	-2.217345	0.860187	-3.174084
Fe	-0.014926	-0.472156	0.117721
P	1.588677	-1.479432	-1.381025
C	2.374378	-0.496802	-2.715424
C	3.034003	-1.108594	-3.798123
C	3.605159	-0.329513	-4.808699
C	3.518136	1.063245	-4.753414
C	2.859864	1.678653	-3.686856
C	2.286719	0.902506	-2.676096
P	1.457012	0.894002	1.584090
C	2.898340	1.774077	0.887828
C	3.114635	3.087576	1.114018
C	4.245030	3.722690	0.580299
C	5.171273	2.987100	-0.169084
C	4.985020	1.672213	-0.360539
C	3.856550	1.039964	0.175573
P	-1.578627	0.582587	1.623835



C	-2.698091	1.921347	1.079651
C	-2.586915	2.471649	-0.199596
C	-3.452376	3.494142	-0.597083
C	-4.418873	3.963736	0.293860
C	-4.506127	3.415079	1.577971
C	-3.672517	2.432657	1.961052
C	0.485565	2.095945	2.616441
C	-0.769964	1.363607	3.115286
C	2.369474	-0.104450	2.827044
C	3.020452	0.515083	3.910936
C	3.742485	-0.266361	4.823759
C	3.831228	-1.597420	4.650161
C	3.238717	-2.192370	3.597912
C	2.505764	-1.434842	2.670139
C	-2.736677	-0.654219	2.332517
C	-2.282160	-1.563094	3.305944
C	-3.158938	-2.530983	3.814597
C	-4.424872	-2.597863	3.365159
C	-4.863687	-1.744847	2.420701
C	-4.009056	-0.764403	1.890724
C	0.614545	-2.699710	-2.434881
C	-0.611777	-1.979922	-3.000585
C	2.962450	-2.595525	-0.878646
C	2.656552	-3.754185	-0.147503
C	3.681130	-4.598908	0.287847
C	5.014210	-4.287011	0.001234
C	5.322521	-3.176257	-0.687012
C	4.317897	-2.309211	-1.136226
F	0.485564	3.043309	-0.209365
B	0.124246	4.431754	-0.129575
F	-0.586691	4.571988	1.092294
F	1.272137	5.210339	-0.108599
F	-0.688595	4.751365	-1.205969
H	0.089378	-2.061253	0.820768
H	-0.093931	-1.620447	1.437792
H	-0.047716	0.684827	-0.760027
H	2.088652	-1.932723	1.816004
H	3.336321	-3.261589	3.457453
H	4.395714	-2.194041	5.355759
H	4.238103	0.204741	5.663036
H	2.996108	1.587204	4.041952
H	1.632349	-3.995795	0.103786
H	3.443472	-5.490031	0.854182
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H	6.359689	-2.942333	-0.891237
H	4.616325	-1.412099	-1.657845
H	-1.913197	-2.989324	0.907062
H	-3.396785	-4.886352	1.379302
H	-4.913948	-5.716205	-0.307695
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H	-3.559687	-2.791235	-3.069709
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H	-5.940487	0.873105	-2.228360
H	-2.769221	2.489925	-4.466988
H	-1.171939	0.919121	-3.444010
H	-3.768713	2.025476	2.959540
H	-1.820426	2.134695	-0.874326
H	-3.368221	3.926474	-1.585359
H	-5.093165	4.755556	-0.005451
H	-5.252759	3.786711	2.268168

H	2.432746	3.673346	1.711159
H	4.405201	4.779035	0.753294
H	6.044589	3.476991	-0.580284
H	5.709426	1.096655	-0.922558
H	3.732838	-0.020296	0.056096
H	-1.259007	-1.545119	3.654552
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H	-5.094596	-3.351726	3.759512
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H	-5.881281	-1.819629	2.058950
H	3.135011	-2.183351	-3.851721
H	4.119811	-0.806232	-5.632805
H	3.962594	1.665194	-5.535421
H	2.794004	2.758041	-3.641837
H	1.787799	1.399753	-1.859297
H	1.042674	2.515763	3.449411
H	0.195153	2.908711	1.946941
H	-0.496758	0.585763	3.829357
H	-1.441293	2.056930	3.616869
H	1.203919	-3.167340	-3.220197
H	0.281671	-3.499755	-1.767720
H	-1.225513	-2.647150	-3.601421
H	-0.292667	-1.158806	-3.641370

$(\mathbf{1}^{+},BF_4^{-})_b$

C	-3.634003	2.771820	0.866018
C	-2.734583	2.002805	0.110823
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C	-3.877009	2.775591	-1.880016
C	-4.736679	3.486889	-1.126465
C	-4.637156	3.503087	0.216314
P	-1.399231	1.066319	0.933085
C	-2.284804	0.109218	2.214299
C	-3.637579	-0.241085	2.073882
C	-4.261619	-1.012285	3.063388
C	-3.575282	-1.428649	4.144239
C	-2.273832	-1.122758	4.303537
C	-1.597839	-0.355473	3.345482
Fe	0.008356	-0.336002	-0.335646
P	1.660967	1.132916	0.596639
C	2.486004	0.893927	2.215097
C	3.313703	1.890747	2.763045
C	3.935853	1.691171	3.998916
C	3.731409	0.501255	4.701377
C	2.900525	-0.487591	4.170292
C	2.277906	-0.289614	2.935052
P	1.457358	-2.019637	-1.098841
C	2.520794	-2.649553	0.251128
C	3.828921	-2.323180	0.334103
C	4.609145	-2.779016	1.404964
C	4.032096	-3.574559	2.401332
C	2.731699	-3.898086	2.332906
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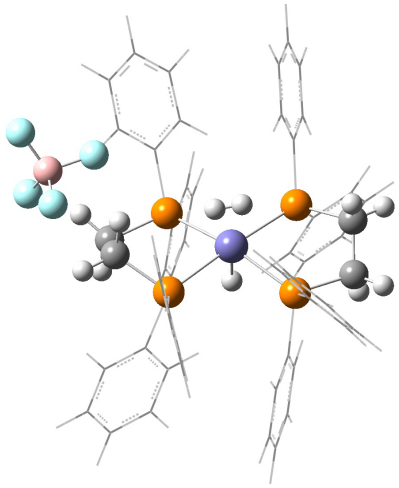

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C	-0.718176	-3.063813	-2.427696
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C	3.546945	-2.615534	-2.896355
C	4.453675	-2.297166	-3.916510
C	4.449966	-1.067068	-4.462022
C	3.578231	-0.131480	-4.039657
C	2.658391	-0.421608	-3.018437
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C	-4.196092	-1.115080	-1.600968
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C	5.202110	2.560449	-2.022276
C	3.973287	3.064285	-2.221969
C	2.895307	2.659318	-1.423950
F	0.830252	5.442032	-0.127198
B	-0.541918	5.466637	0.165424
F	-0.713763	5.273653	1.559816
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F	-1.149233	4.354265	-0.496745
H	0.013116	0.947149	-1.530924
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H	3.586609	0.853919	-4.488024
H	5.154439	-0.827142	-5.248490
H	5.159130	-3.041755	-4.262632
H	3.565783	-3.602887	-2.453451
H	4.566588	0.462118	0.569539
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H	6.023204	2.878927	-2.651723
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H	-1.740257	-1.479628	5.175224
H	-0.547429	-0.144996	3.483177
H	-3.549519	-4.023732	-1.674298
H	-1.289294	-2.547957	1.688334
H	-2.370399	-4.219633	3.123842
H	-4.035009	-5.785974	2.153823
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H	5.655508	-2.509187	1.465775
H	4.634473	-3.921868	3.230936

H	2.282903	-4.504040	3.109579
H	0.897042	-3.690087	1.244859
H	-1.793516	-0.733022	-3.916555
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H	-6.239023	-0.483980	-1.875257
H	3.492004	2.815053	2.229840
H	4.578050	2.458634	4.411107
H	4.213691	0.347056	5.657843
H	2.736055	-1.407360	4.716633
H	1.627799	-1.057316	2.552173
H	1.201062	-4.103121	-2.464184
H	0.352512	-4.207588	-0.932060
H	-0.468904	-2.493062	-3.323316
H	-1.348061	-3.898980	-2.727366
H	1.369535	3.487973	1.417142
H	0.380724	3.139554	0.034102
H	-1.052342	3.304323	1.936720
H	-0.174929	2.041042	2.827060

2^{+}

Ru	-0.046051	-1.199190	-0.916150
P	1.857783	0.087462	-0.091844
P	-1.878402	0.066414	-0.023640
C	0.085664	-3.115007	-2.131515
C	1.047939	-3.204335	-1.103260
H	2.107655	-3.335712	-1.252482
C	0.349528	-3.183870	0.154383
H	0.778694	-3.302829	1.136074
C	-1.210586	-3.022687	-1.535256
H	-2.150649	-2.995610	-2.063158
C	-1.032991	-3.102188	-0.120675
H	-1.813194	-3.118065	0.624252
H	0.294381	-3.100193	-3.190597
C	-1.976456	1.868896	-0.372836
C	-3.427236	-0.592135	-0.741260
C	-2.045548	-0.155868	1.782127
C	3.289521	-0.050274	-1.212393
C	2.620870	-0.498833	1.473001
C	1.571263	1.890641	0.058678
C	-1.504602	2.364292	-1.601207
C	-1.588855	3.725821	-1.904479
C	-2.149753	4.613613	-0.987142
C	-2.620921	4.140457	0.237358
C	-2.531039	2.779699	0.547391
H	-1.079579	1.706680	-2.338872
H	-1.219283	4.092007	-2.853564
H	-2.212722	5.668164	-1.221884
H	-3.046046	4.831039	0.954230
H	-2.882478	2.467378	1.512938
C	-3.814988	-0.198670	-2.032954
C	-4.968893	-0.725971	-2.619819
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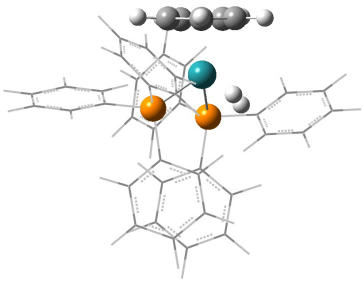

C	-5.344234	-2.091314	-0.661390
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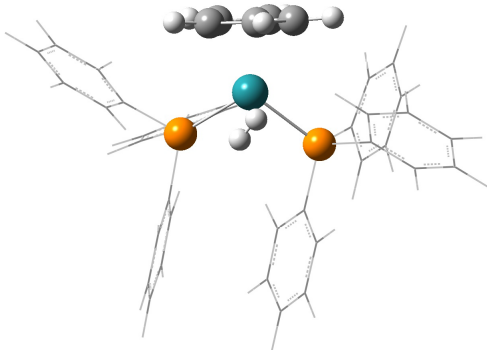
H	-5.263094	-0.410133	-3.612396
H	-6.627447	-2.078241	-2.389376
H	-5.928329	-2.836134	-0.136447
H	-3.894875	-1.939726	0.897459
C	-3.240324	0.140779	2.461343
C	-3.336496	-0.062090	3.841326
C	-2.247017	-0.573185	4.551359
C	-1.064010	-0.890821	3.879766
C	-0.968398	-0.691241	2.500199
H	-4.099660	0.520065	1.923322
H	-4.257325	0.172647	4.359290
H	-2.322204	-0.730338	5.619555
H	-0.222129	-1.295912	4.426434
H	-0.054042	-0.954566	1.992711
C	2.802724	0.336185	2.592681
C	3.382997	-0.161888	3.763403
C	3.815839	-1.486866	3.823281
C	3.690033	-2.309147	2.703668
C	3.109702	-1.813390	1.533306
H	2.534922	1.376827	2.576707
H	3.509610	0.485667	4.621485
H	4.268393	-1.869253	4.728999
H	4.051951	-3.328589	2.738020
H	3.064168	-2.453561	0.667483
C	3.183798	-0.749866	-2.422690
C	4.290579	-0.863639	-3.269520
C	5.509491	-0.281292	-2.912209
C	5.623588	0.414798	-1.706205
C	4.519138	0.529071	-0.857215
H	2.253150	-1.209759	-2.716318
H	4.203327	-1.404678	-4.202862
H	6.365138	-0.370271	-3.568942
H	6.567754	0.865338	-1.428874
H	4.620153	1.072079	0.073929
C	0.769884	2.391657	1.096795
C	0.572155	3.767567	1.241712
C	1.126234	4.655055	0.318130
C	1.877513	4.166166	-0.751972
C	2.096014	2.791718	-0.886276
H	0.312266	1.719465	1.808529
H	-0.028460	4.143756	2.059612
H	0.957942	5.719181	0.421219
H	2.288506	4.852513	-1.480854
H	2.663125	2.443366	-1.737268
H	-0.478549	-0.430704	-2.397091
H	0.292747	-0.136139	-2.268106

TS for rotation of coordinated H_2 in 2^+

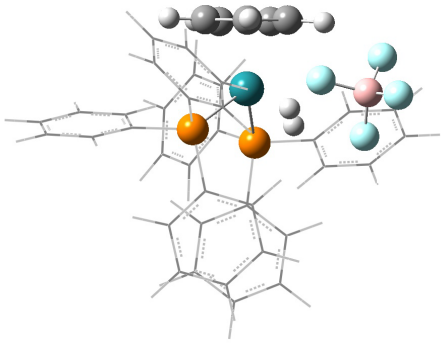
Ru	-0.049529	-1.234531	-0.887089
P	1.883919	0.050529	-0.111718
P	-1.894547	0.081301	-0.027725
C	0.048995	-3.188846	-2.047705
C	0.970764	-3.270922	-0.976037
H	2.031022	-3.440775	-1.074854
C	0.226903	-3.190760	0.248997
H	0.611708	-3.292851	1.250430
C	-1.262909	-3.035325	-1.512202



H	-2.179513	-2.999980	-2.078523
C	-1.139246	-3.061561	-0.088115
H	-1.947551	-3.024769	0.625869
H	0.300351	-3.226477	-3.097097
C	-2.035044	1.855870	-0.508070
C	-3.465352	-0.670100	-0.611820
C	-1.976642	0.006692	1.796917
C	3.341316	-0.170348	-1.184967
C	2.606284	-0.422552	1.507917
C	1.612284	1.860377	-0.108320
C	-1.866902	2.235842	-1.853247
C	-1.989548	3.572512	-2.242529
C	-2.286150	4.552952	-1.297455
C	-2.447036	4.198843	0.040950
C	-2.310118	2.864779	0.437167
H	-1.638657	1.512576	-2.617020
H	-1.855793	3.847411	-3.280823
H	-2.380324	5.587740	-1.600086
H	-2.655421	4.962735	0.778917
H	-2.385187	2.654025	1.488224
C	-3.836953	-0.550612	-1.962147
C	-5.012082	-1.141926	-2.434748
C	-5.820045	-1.881821	-1.571246
C	-5.443648	-2.046140	-0.238108
C	-4.269264	-1.455944	0.237762
H	-3.215411	-0.023293	-2.664938
H	-5.289709	-1.036016	-3.475548
H	-6.727026	-2.343535	-1.939499
H	-6.055055	-2.644231	0.425257
H	-3.984794	-1.652663	1.259629
C	-3.099761	0.464128	2.509158
C	-3.130397	0.385146	3.904677
C	-2.046185	-0.158316	4.598760
C	-0.934475	-0.630569	3.896768
C	-0.904947	-0.554860	2.501906
H	-3.950199	0.879735	1.983504
H	-3.995320	0.743568	4.447556
H	-2.069932	-0.218552	5.679088
H	-0.096461	-1.058171	4.432185
H	-0.046356	-0.933913	1.972500
C	2.889637	0.516158	2.518855
C	3.431549	0.102299	3.739636
C	3.728555	-1.244007	3.954788
C	3.508668	-2.174210	2.938649
C	2.966544	-1.762243	1.718422
H	2.736573	1.571055	2.373731
H	3.636017	0.829946	4.514448
H	4.152015	-1.561871	4.898716
H	3.769442	-3.213503	3.091233
H	2.851361	-2.488890	0.931009
C	3.270059	-0.966267	-2.336513
C	4.396390	-1.134644	-3.147819
C	5.600671	-0.509687	-2.813915
C	5.680173	0.284278	-1.667174
C	4.555948	0.453218	-0.853986
H	2.352102	-1.458469	-2.612498
H	4.335397	-1.750395	-4.035850
H	6.471408	-0.640678	-3.443229
H	6.612599	0.769012	-1.408382
H	4.630302	1.073747	0.029980
C	0.870522	2.461169	0.920243

C	0.697512	3.847915	0.952211
C	1.196721	4.639741	-0.083119
C	1.877675	4.045548	-1.147020
C	2.083777	2.662858	-1.162965
H	0.446999	1.860352	1.713482
H	0.152576	4.305449	1.767722
H	1.042542	5.710810	-0.068446
H	2.247472	4.656685	-1.960094
H	2.602046	2.228093	-2.006036
H	0.273212	-0.585163	-2.486236
H	-0.149186	0.011200	-2.138121

(2^{+},BF_4^{-})



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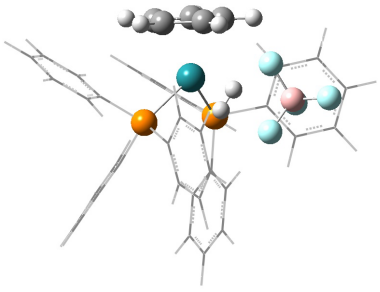
P	-1.776111	-0.664714	0.045146
C	0.921467	1.344842	-2.952513
C	0.362838	0.047667	-3.241202
H	0.890192	-0.825688	-3.589656
C	-1.034282	0.139627	-3.074261
H	-1.729690	-0.666193	-3.251536
C	-0.136459	2.211636	-2.599097
H	-0.045821	3.231808	-2.248229
C	-1.351895	1.466545	-2.639347
H	-2.324924	1.874001	-2.418751
H	1.956709	1.633564	-3.040083
C	-1.849475	-0.668552	1.883620
C	-3.413730	-0.012023	-0.454961
C	-1.787865	-2.410469	-0.496396
C	3.203308	1.061507	0.156815
C	2.875525	-1.547000	-0.821934
C	1.693809	-0.774010	1.781486
C	-1.563009	0.511866	2.591740
C	-1.633244	0.545595	3.986880
C	-1.994969	-0.598572	4.697041
C	-2.278115	-1.779932	4.011898
C	-2.198509	-1.820072	2.616252
H	-1.300642	1.418671	2.075177
H	-1.410184	1.462300	4.517185
H	-2.048332	-0.572075	5.777609
H	-2.544912	-2.672094	4.563568
H	-2.391151	-2.761725	2.135890
C	-3.955020	1.107947	0.198908
C	-5.178481	1.646986	-0.208815
C	-5.868247	1.084513	-1.283883
C	-5.329965	-0.012254	-1.958655
C	-4.106316	-0.553308	-1.554053
H	-3.434442	1.579401	1.017043
H	-5.587919	2.507203	0.304917
H	-6.813914	1.504988	-1.600612
H	-5.856669	-0.438527	-2.802621
H	-3.701900	-1.383194	-2.114821
C	-2.905305	-3.240841	-0.301491
C	-2.888910	-4.562544	-0.756800
C	-1.764241	-5.060449	-1.420124
C	-0.658603	-4.234017	-1.636275
C	-0.674830	-2.911918	-1.184163
H	-3.788802	-2.864597	0.198358
H	-3.749810	-5.199228	-0.599227
H	-1.752537	-6.083540	-1.772875
H	0.209393	-4.615620	-2.158369

H	0.180671	-2.279975	-1.371360
C	3.274088	-2.742278	-0.192232
C	3.994464	-3.710675	-0.898420
C	4.352211	-3.487743	-2.228498
C	4.010408	-2.284949	-2.846745
C	3.290066	-1.316471	-2.142736
H	3.072998	-2.932559	0.846868
H	4.288715	-4.629650	-0.407947
H	4.913765	-4.236497	-2.771983
H	4.313856	-2.096793	-3.868500
H	3.079690	-0.376271	-2.625094
C	2.931303	2.368210	-0.270631
C	3.914837	3.357778	-0.183931
C	5.177113	3.047826	0.328971
C	5.456976	1.747040	0.755554
C	4.475082	0.755822	0.669373
H	1.963868	2.628090	-0.668276
H	3.697754	4.365389	-0.514239
H	5.937476	3.815083	0.396222
H	6.434127	1.507007	1.154162
H	4.703028	-0.246712	1.008353
C	1.066767	-1.999275	2.057590
C	0.922353	-2.441904	3.375320
C	1.345351	-1.636763	4.434047
C	1.912553	-0.387783	4.174971
C	2.082773	0.045824	2.856738
H	0.712136	-2.626507	1.251905
H	0.461942	-3.400655	3.575633
H	1.216377	-1.972452	5.454741
H	2.218818	0.246715	4.996474
H	2.506909	1.025310	2.688552
H	-0.581691	1.866510	-0.013670
H	0.144125	1.628169	0.316961
B	-0.761607	4.311434	0.232372
F	0.095180	4.653280	-0.833933
F	-1.431596	5.408806	0.717320
F	-1.703469	3.347537	-0.275114
F	-0.013733	3.672649	1.240404

TS for rotation of coordinated H_2 in the (2^+,BF_4^-) ion pair

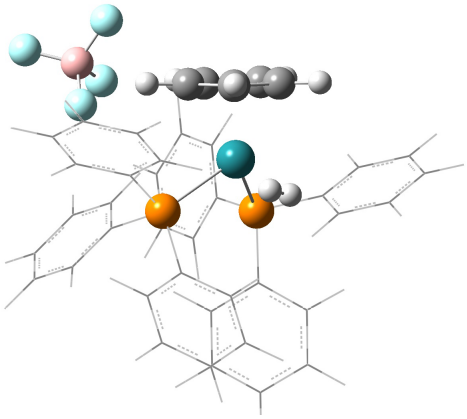
Ru	0.040681	0.368334	-1.240320
P	1.745953	-0.711224	0.086182
P	-1.982091	-0.071977	0.008463
C	1.118936	1.249066	-2.988210
C	0.990458	-0.143655	-3.265042
H	1.799172	-0.846394	-3.393204
C	-0.385791	-0.466822	-3.354085
H	-0.792237	-1.431004	-3.609828
C	-0.201717	1.802420	-2.958465
H	-0.424365	2.830007	-2.719348
C	-1.120428	0.754948	-3.168091
H	-2.191665	0.869870	-3.222359
H	2.024383	1.818346	-2.851582
C	-2.420786	1.463457	0.897645
C	-3.397250	-0.448453	-1.082952
C	-2.183360	-1.454190	1.183707
C	3.342776	0.183232	0.043308
C	2.230366	-2.355526	-0.539673
C	1.359978	-0.933369	1.864141
C	-2.688131	2.623996	0.153037



C	-2.947481	3.836067	0.798730
C	-2.903929	3.908504	2.192852
C	-2.586304	2.772093	2.940506
C	-2.330840	1.557696	2.296835
H	-2.695003	2.588748	-0.929323
H	-3.168294	4.721898	0.217546
H	-3.097288	4.848847	2.692491
H	-2.523679	2.835163	4.019168
H	-2.042918	0.706633	2.895322
C	-4.609696	0.262492	-1.026076
C	-5.670169	-0.085514	-1.868659
C	-5.539756	-1.156902	-2.755275
C	-4.353847	-1.893308	-2.788744
C	-3.292826	-1.548512	-1.947400
H	-4.759232	1.067022	-0.323085
H	-6.598505	0.469373	-1.825959
H	-6.362868	-1.426058	-3.404440
H	-4.259135	-2.736449	-3.460663
H	-2.389492	-2.144613	-1.963303
C	-3.288668	-1.500187	2.051096
C	-3.483781	-2.601835	2.889502
C	-2.604402	-3.685674	2.835290
C	-1.542876	-3.675298	1.928048
C	-1.344184	-2.569149	1.096663
H	-4.005135	-0.689502	2.073237
H	-4.325336	-2.621655	3.569714
H	-2.757805	-4.541198	3.480095
H	-0.876246	-4.525591	1.864474
H	-0.543371	-2.587991	0.379473
C	3.432505	-2.956292	-0.128777
C	3.799561	-4.209918	-0.626742
C	2.972461	-4.870177	-1.539052
C	1.777064	-4.277248	-1.953399
C	1.408433	-3.023677	-1.457162
H	4.084063	-2.457439	0.576436
H	4.725468	-4.669205	-0.305651
H	3.256940	-5.841052	-1.923527
H	1.134233	-4.790168	-2.656991
H	0.472954	-2.586058	-1.773577
C	3.975869	0.639971	1.215177
C	5.199208	1.313271	1.142445
C	5.811768	1.523295	-0.094098
C	5.207576	1.048618	-1.259147
C	3.985146	0.375050	-1.189499
H	3.541288	0.485444	2.188791
H	5.674440	1.669569	2.047296
H	6.759417	2.043295	-0.148169
H	5.690895	1.194030	-2.216576
H	3.556100	-0.017289	-2.097336
C	0.904202	0.168642	2.605288
C	0.554688	0.025954	3.950710
C	0.651292	-1.220606	4.570303
C	1.102768	-2.324743	3.845727
C	1.453647	-2.185997	2.499395
H	0.823129	1.142556	2.148177
H	0.203399	0.882715	4.511169
H	0.374957	-1.331378	5.610770
H	1.169507	-3.293317	4.324071
H	1.769894	-3.067253	1.964918
H	0.099704	1.550462	0.048100
H	0.517974	1.893451	-0.559266

B	1.322776	3.890810	0.166327
F	2.298464	2.872220	0.229961
F	1.869816	5.136133	0.348956
F	0.727740	3.782169	-1.132972
F	0.323756	3.603156	1.113670

(2^{+},BF_4^-)$_b$

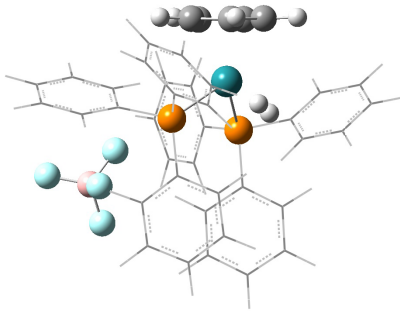


Ru	0.097672	-0.119276	-1.515286
P	2.104880	-0.009399	-0.073649
P	-1.529229	0.970725	-0.075057
C	0.750790	-2.061222	-2.484991
C	-0.285763	-2.367921	-1.539706
H	-0.258341	-3.037190	-0.691004
C	-1.467078	-1.728148	-1.986920
H	-2.409384	-1.830813	-1.471818
C	0.212423	-1.210873	-3.477295
H	0.740974	-0.810921	-4.328959
C	-1.165610	-0.979843	-3.158564
H	-1.861854	-0.417281	-3.759129
H	1.759825	-2.442766	-2.482133
C	-1.416617	2.799814	0.018739
C	-3.212607	0.755699	-0.743133
C	-1.572653	0.367202	1.646198
C	3.635025	-0.246455	-1.040146
C	2.308676	-1.321593	1.196741
C	2.389017	1.599622	0.765006
C	-0.238947	3.460522	-0.358616
C	-0.153254	4.854436	-0.303178
C	-1.255454	5.607301	0.104159
C	-2.447900	4.966075	0.443621
C	-2.533080	3.571651	0.391751
H	0.620482	2.907655	-0.689539
H	0.768409	5.350264	-0.579573
H	-1.189554	6.686814	0.144659
H	-3.309712	5.549800	0.740163
H	-3.477695	3.102233	0.629978
C	-3.483629	1.223359	-2.037434
C	-4.760958	1.085647	-2.587356
C	-5.781370	0.488437	-1.843997
C	-5.525957	0.034251	-0.547932
C	-4.249159	0.171084	0.005248
H	-2.703589	1.696686	-2.620514
H	-4.959897	1.444237	-3.588956
H	-6.770666	0.382244	-2.269862
H	-6.318911	-0.422551	0.029979
H	-4.084430	-0.182479	1.011771
C	-2.240893	1.058958	2.671580
C	-2.222758	0.568527	3.981213
C	-1.541870	-0.614376	4.277806
C	-0.881018	-1.309454	3.263789
C	-0.895539	-0.817171	1.956528
H	-2.780318	1.969071	2.474966
H	-2.738632	1.105724	4.766505
H	-1.529736	-0.993630	5.291351
H	-0.358339	-2.229800	3.489093
H	-0.389147	-1.365296	1.178856
C	2.605652	-1.030766	2.542821
C	2.740368	-2.060723	3.478793
C	2.607366	-3.391472	3.081185
C	2.365931	-3.694638	1.741181
C	2.234169	-2.666880	0.803766

H	2.764881	-0.022810	2.884143
H	2.957652	-1.826079	4.512837
H	2.712397	-4.187435	3.806899
H	2.291828	-4.727206	1.425340
H	2.095191	-2.928128	-0.230905
C	3.605575	-0.190853	-2.440163
C	4.780015	-0.364314	-3.178517
C	5.993935	-0.583689	-2.522589
C	6.035566	-0.622374	-1.126758
C	4.862472	-0.449834	-0.386506
H	2.682876	-0.000195	-2.963690
H	4.749721	-0.322764	-4.259585
H	6.902658	-0.716167	-3.095348
H	6.977345	-0.782324	-0.617994
H	4.913995	-0.468639	0.694299
C	1.580023	1.981795	1.848299
C	1.742263	3.229138	2.456528
C	2.702742	4.120457	1.976860
C	3.499528	3.764876	0.887185
C	3.341585	2.515748	0.278725
H	0.834354	1.309739	2.236783
H	1.116878	3.506743	3.295097
H	2.823575	5.089462	2.443384
H	4.233462	4.462719	0.505425
H	3.949723	2.288278	-0.584477
H	0.045165	1.405989	-2.329727
H	0.875087	1.267383	-2.243881
B	-2.469271	-3.737245	0.448003
F	-3.344600	-4.444708	1.241779
F	-2.505996	-4.168465	-0.887877
F	-2.812828	-2.348680	0.454420
F	-1.139719	-3.856821	0.923369

$(\mathbf{2}^{+},BF_4^{-})_c$

Ru	0.057359	-1.736437	-0.612926
P	-1.929713	-0.437108	0.059803
P	1.883193	-0.350013	0.171634
C	-0.912093	-2.711485	-2.465187
C	0.028723	-1.734669	-2.929458
H	-0.168761	-0.895531	-3.575508
C	1.312419	-2.141165	-2.499144
H	2.230169	-1.625722	-2.733070
C	-0.200237	-3.701384	-1.752723
H	-0.619921	-4.583681	-1.295149
C	1.185071	-3.338769	-1.745204
H	1.990784	-3.910865	-1.313075
H	-1.972585	-2.713682	-2.663267
C	1.858110	0.323954	1.880287
C	3.325222	-1.485813	0.215948
C	2.352090	0.961893	-1.003805
C	-3.394571	-1.529971	0.122733
C	-2.545037	0.904220	-1.020897
C	-1.870614	0.235028	1.758351
C	1.240428	-0.418863	2.902264
C	1.280984	0.016653	4.229520
C	1.922764	1.211383	4.553819
C	2.531795	1.965931	3.551164
C	2.509087	1.522795	2.225115
H	0.724166	-1.338836	2.683657
H	0.801517	-0.566897	5.004805



H	1.944619	1.554016	5.580120
H	3.030665	2.893075	3.802294
H	3.006519	2.127929	1.490881
C	3.425456	-2.437729	1.245949
C	4.491845	-3.340528	1.282463
C	5.461014	-3.320316	0.279186
C	5.356868	-2.405732	-0.769184
C	4.292188	-1.500880	-0.808663
H	2.678298	-2.497789	2.021187
H	4.561538	-4.062613	2.085778
H	6.284042	-4.022662	0.306225
H	6.095685	-2.405456	-1.560169
H	4.222417	-0.841135	-1.659356
C	3.606180	1.596871	-0.950849
C	3.958044	2.546438	-1.914666
C	3.070350	2.857401	-2.947454
C	1.830137	2.218867	-3.016173
C	1.473318	1.277366	-2.046370
H	4.325150	1.334560	-0.185753
H	4.924873	3.030557	-1.868787
H	3.344357	3.590195	-3.695198
H	1.138900	2.462351	-3.812563
H	0.498733	0.815768	-2.091183
C	-3.159875	2.058050	-0.494271
C	-3.671107	3.041247	-1.347080
C	-3.600559	2.873184	-2.730889
C	-3.044905	1.708198	-3.261965
C	-2.539450	0.722072	-2.410145
H	-3.275348	2.198603	0.569256
H	-4.130914	3.929527	-0.933642
H	-3.998156	3.633680	-3.390320
H	-3.022829	1.559718	-4.333786
H	-2.179049	-0.195761	-2.836432
C	-3.244559	-2.920821	0.040304
C	-4.361305	-3.759521	0.101425
C	-5.637653	-3.215294	0.259841
C	-5.796462	-1.832040	0.367789
C	-4.680719	-0.992033	0.306388
H	-2.267728	-3.362713	-0.047093
H	-4.235681	-4.832481	0.034702
H	-6.501478	-3.865424	0.309964
H	-6.783816	-1.410395	0.504801
H	-4.824738	0.073477	0.412949
C	-1.216240	1.448253	2.001236
C	-1.211682	2.014627	3.278343
C	-1.827922	1.347275	4.338700
C	-2.440094	0.110655	4.121144
C	-2.459144	-0.447364	2.838659
H	-0.723288	1.956877	1.194207
H	-0.715826	2.961533	3.448014
H	-1.814893	1.778888	5.330967
H	-2.900701	-0.416286	4.946667
H	-2.930805	-1.410054	2.701302
H	0.414991	-2.596992	0.824100
H	-0.400892	-2.407035	0.923390
B	0.174017	4.023597	-0.426135
F	-0.568881	3.106575	-1.214151
F	1.167452	3.279058	0.266111
F	0.784246	4.963010	-1.250262
F	-0.675403	4.627512	0.501408

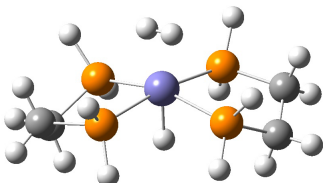
QM calculations on the simplified model

BF_4^-

B	-0.000346	-0.000031	0.000197
F	-0.736300	1.137425	0.379936
F	-0.865618	-0.947342	-0.577480
F	0.618245	-0.559183	1.133358
F	0.983866	0.369117	-0.935923

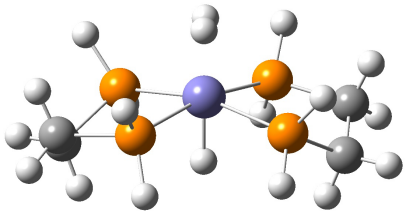
$1s^+$

Fe	0.000008	0.000000	-0.362718
H	-0.319188	-0.224836	-2.074321
H	-0.000098	-0.000117	1.155267
P	-1.624744	-1.573125	0.006313
H	-2.297514	-2.275752	-1.019015
H	-1.327302	-2.659556	0.851206
P	-1.734225	1.519538	-0.150878
H	-2.111368	2.461105	-1.131346
H	-1.656529	2.382266	0.959519
P	1.624785	1.573162	0.006092
H	2.297548	2.275613	-1.019357
H	1.327487	2.659707	0.850894
P	1.734196	-1.519560	-0.150963
H	1.656499	-2.382575	0.959206
H	2.111386	-2.460866	-1.131662
C	-3.322257	0.591191	0.134787
H	-3.743056	0.380339	-0.851056
H	-4.040473	1.202637	0.679139
C	-3.018446	-0.714387	0.876687
H	-3.900642	-1.350551	0.936276
H	-2.667394	-0.510586	1.889941
C	3.322231	-0.591237	0.134854
H	4.040344	-1.202673	0.679355
H	3.743175	-0.380516	-0.850955
C	3.018425	0.714434	0.876586
H	2.667267	0.510754	1.889829
H	3.900648	1.350558	0.936190
H	0.319101	0.224812	-2.074367



TS for rotation of coordinated H_2 in $1s^+$

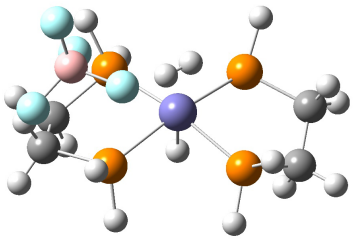
Fe	0.000031	-0.000107	-0.365012
H	0.065185	-0.383939	-2.082914
H	0.000458	-0.000046	1.152564
P	-1.651823	-1.565440	-0.038721
H	-2.337197	-2.221714	-1.086016
H	-1.378084	-2.684968	0.771234
P	-1.711675	1.529446	-0.110277
H	-2.080684	2.502200	-1.063450
H	-1.607025	2.364044	1.019096
P	1.651712	1.565402	-0.039031
H	2.337249	2.221440	-1.086370
H	1.377629	2.685187	0.770477
P	1.711871	-1.529483	-0.110463
H	1.607287	-2.364683	1.018459
H	2.081533	-2.501621	-1.064039
C	-3.313317	0.621476	0.162527
H	-3.745456	0.447521	-0.825505
H	-4.015146	1.230791	0.730286



C	-3.028887	-0.710558	0.863292
H	-3.921663	-1.332985	0.907357
H	-2.671133	-0.543301	1.880834
C	3.313286	-0.621226	0.162961
H	4.014991	-1.230485	0.730943
H	3.745718	-0.447280	-0.824945
C	3.028602	0.710838	0.863535
H	2.670606	0.543709	1.881008
H	3.921309	1.333360	0.907709
H	-0.065754	0.383527	-2.082896

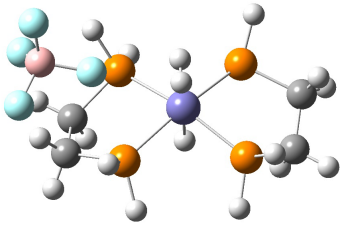
($1s^+$,BF_4^-)

Fe	-0.807025	0.128823	-0.018248
H	-0.328461	-0.900003	-1.333429
H	-1.515219	1.067567	0.968827
P	0.318481	2.019612	-0.668869
H	1.216902	2.089101	-1.745163
H	-0.468459	3.159007	-0.959414
P	0.816126	0.005469	1.613612
H	1.710240	-1.067617	1.746031
H	0.293324	0.070038	2.924965
P	-2.127556	-1.434618	0.983869
H	-2.159306	-2.805332	0.631756
H	-2.104293	-1.589983	2.384847
P	-2.636855	0.578419	-1.302521
H	-3.202155	1.861469	-1.152376
H	-2.716779	0.495693	-2.711803
C	1.954623	1.470999	1.531721
H	2.821123	1.110515	0.982986
H	2.263354	1.766446	2.534081
C	1.271547	2.631088	0.804612
H	1.992610	3.394748	0.514214
H	0.517585	3.092554	1.446056
C	-4.034434	-0.554032	-0.806266
H	-5.004135	-0.104158	-1.016189
H	-3.938401	-1.447166	-1.428716
C	-3.890823	-0.926071	0.673305
H	-4.066621	-0.052804	1.304272
H	-4.595439	-1.707776	0.955436
H	0.318089	-0.986414	-0.907974
B	3.025044	-1.099807	-0.680667
F	2.011153	-2.064692	-0.473158
F	3.713910	-0.897106	0.525000
F	2.355013	0.134093	-0.995185
F	3.860486	-1.456893	-1.709128



TS for rotation of coordinated H_2 in the ($1s^+$,BF_4^-) ion pair

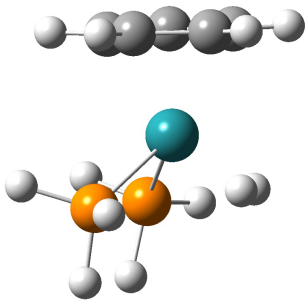
Fe	0.964958	0.007508	-0.100404
H	0.337689	0.195779	-1.730871
H	1.499069	0.195140	1.323742
P	2.660394	1.466868	-0.531692
H	3.038501	1.954585	-1.807052
H	2.709623	2.690306	0.166399
P	2.589901	-1.599964	-0.201192
H	2.644178	-2.702047	-1.084594
H	2.823958	-2.302449	0.998098
P	-0.561948	-1.376988	0.912219
H	-1.558332	-2.103225	0.245451
H	-0.004876	-2.400210	1.715856
P	-0.536336	1.653311	0.485927



H	0.065178	2.730839	1.179013
H	-1.304574	2.386612	-0.434251
C	4.238584	-0.794588	-0.542206
H	4.350022	-0.773441	-1.629148
H	5.061077	-1.381089	-0.134470
C	4.231670	0.633165	0.013321
H	5.114671	1.187235	-0.303707
H	4.200504	0.618287	1.104108
C	-1.804113	1.024774	1.690223
H	-1.881045	1.721763	2.524178
H	-2.749828	1.017490	1.154513
C	-1.455780	-0.378864	2.194337
H	-0.762153	-0.324310	3.034980
H	-2.360187	-0.902513	2.497174
H	0.329405	-0.574497	-1.636123
B	-3.463123	-0.165324	-0.865615
F	-3.614897	-1.024050	0.242201
F	-4.046172	-0.686102	-1.995387
F	-2.039195	-0.024460	-1.076587
F	-3.951793	1.105927	-0.543303

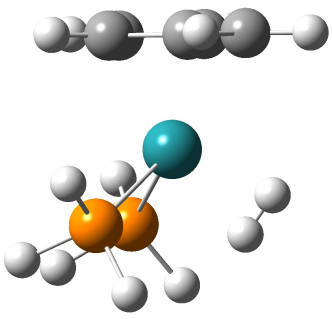
$2s^+$

Ru	0.032315	0.000001	-0.330019
P	1.570795	-1.669218	0.164143
P	1.570771	1.669236	0.164138
H	1.615103	-2.081544	1.509234
H	1.417286	-2.921696	-0.458896
H	2.946522	1.468759	-0.062764
H	1.417408	2.921599	-0.459160
H	2.946506	-1.468822	-0.063053
H	1.614843	2.081791	1.509163
C	-2.107841	0.718872	-0.577987
C	-1.629087	1.153630	0.680063
H	-1.534079	2.181060	0.997957
C	-1.286017	-0.000723	1.457659
H	-0.944579	-0.001354	2.480530
C	-2.108146	-0.717729	-0.578767
H	-2.440394	-1.350684	-1.386395
C	-1.629539	-1.154112	0.678759
H	-1.534979	-2.181938	0.995505
H	-2.439924	1.352853	-1.384875
H	0.477360	0.414904	-2.019481
H	0.477359	-0.414832	-2.019494



TS for rotation of coordinated H_2 in $2s^+$

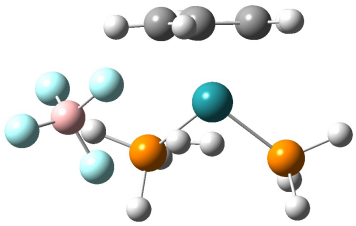
Ru	-0.039816	-0.001809	-0.321650
P	-1.544437	1.715041	0.163807
P	-1.559721	-1.703774	0.164991
H	-0.980672	2.830026	0.810377
H	-2.234374	2.375384	-0.870703
H	-2.390660	-2.234515	-0.839287
H	-0.997597	-2.899004	0.649893
H	-2.627401	1.474534	1.032425



H	-2.532416	-1.488152	1.161404
C	1.897796	-1.141469	-0.088564
C	1.404136	-0.765406	1.202544
H	1.123207	-1.438320	1.998137
C	1.373130	0.652222	1.274017
H	1.074942	1.230518	2.134827
C	2.185416	0.061580	-0.794554
H	2.568121	0.119900	-1.802529
C	1.860645	1.172654	0.027499
H	2.002600	2.211703	-0.222615
H	2.077734	-2.144397	-0.440263
H	-0.931511	-0.007567	-1.958657
H	-0.164422	0.003001	-2.158057

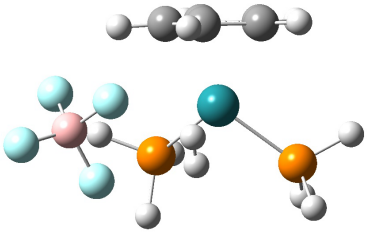
($2s^+$,BF_4^-)

Ru	-0.873644	-0.031527	-0.165961
P	-2.608465	-1.433702	-0.728350
P	0.163633	-1.639561	1.154196
H	1.309887	-1.199875	1.829039
H	-0.628614	-2.147904	2.209773
H	0.593435	-2.850483	0.591129
H	-2.488541	-2.353442	-1.791014
H	-3.816898	-0.824185	-1.126333
H	-3.145188	-2.323721	0.229480
C	-1.682630	2.043521	-0.604508
C	-2.192167	1.608058	0.661809
H	-3.232141	1.463210	0.912612
C	-1.094545	1.418781	1.541184
H	-1.162505	1.107520	2.572396
C	-0.265129	2.116021	-0.485636
H	0.441743	2.338045	-1.268836
C	0.110859	1.727802	0.826026
H	1.126417	1.628764	1.178037
H	-2.266267	2.302720	-1.472960
H	-0.217212	-0.544701	-1.723522
H	0.452694	-0.580912	-1.251749
B	2.937536	-0.036320	-0.291274
F	4.265330	-0.155699	-0.609408
F	2.303491	0.970221	-1.044865
F	2.248548	-1.267048	-0.560253
F	2.760409	0.248928	1.086709



TS for rotation of coordinated H_2 in the ($2s^+$,BF_4^-) ion pair

Ru	-0.846636	-0.045376	-0.143951
P	-2.513969	-1.494922	-0.804602
P	0.209406	-1.559135	1.276602
H	1.362642	-1.066874	1.900104
H	-0.575378	-1.964640	2.381526
H	0.624677	-2.819758	0.823139
H	-2.433700	-2.178100	-2.036593
H	-3.793960	-0.925346	-0.972284
H	-2.896701	-2.597740	-0.007722
C	-1.804271	1.961197	-0.603026
C	-2.231318	1.515072	0.694159
H	-3.246972	1.307604	0.994218
C	-1.086628	1.430691	1.527898
H	-1.087660	1.134522	2.566214
C	-0.394733	2.136556	-0.544408



H	0.256610	2.399714	-1.362948
C	0.064384	1.802548	0.757602
H	1.096706	1.778388	1.071482
H	-2.439544	2.162368	-1.450417
H	0.297275	-0.203079	-1.519476
H	0.162677	-0.966815	-1.325119
B	2.893344	-0.025896	-0.321252
F	4.217519	-0.070378	-0.674526
F	2.163117	0.844011	-1.168770
F	2.302533	-1.321422	-0.417757
F	2.732656	0.414484	1.017123