On the reaction mechanism of redox trans metallation of elemental Yb by $Hg(C_6F_5)_2$ and subsequent reactivity of $Yb(C_6F_5)_2$ with Pyrazole: A DFT investigation†

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Computational details

All the quantum chemical calculations were performed using Gaussian 09 suite software.[1] Unless specified, the B3PW91[2,3] functional was considered in all the geometry optimisations without imposing any constraint and in the gas phase. The gas phase is appropriate in this case since the experiment were carried out in not polar and coordinating solvent (cyclohexane) so that no specific interactions may modify the reaction pathway determined in the gas phase. Two different Stuttgart-Dresden scalar relativistic effective core potentials were used for Yb atoms; both the small core ECP in combination with its adapted basis set[4] and the 4*f*-in-core ECP (augmented by a *f* polarisation function, $\alpha = 1.0$) for the mechanism exploration.[5] The latter was only used to compare the pyrazole activation mechanism obtained with small core RECPs (explicit f) that are reported in the manuscript with the one obtained with a fixed oxidation state (+II), that are not reported in the text. Hg and Fluorine atoms were represented by the Stuttgart-Dresden effective core potential, and their associated basis set [6,7] Carbon, nitrogen and hydrogen atoms were represented by the 6-31G(d,p) basis set.[8] In all the calculations, spin-orbit effects were neglected. The nature of the optimised extrema (minimum or transition state) was confirmed with an analytical frequency calculation. The connectivity in the transition states was verified by following the Intrinsic Reaction Coordinates (IRC). The zero-point energy (ZPE) and entropic contribution were calculated within the harmonic potential approximation. Enthalpies were calculated at 298.15 K and 1 atm. Electron affinities have been computed according to the following the electron convention: $\Delta_f H°$(e-, 0 K) = 0 kcal mol^{-1}. Calculated values correspond to the electronic values at 0 K corrected by the zero-point vibrational energy (ZPVE) in gas phase.[9] Basis Set Superposition Errors (BSSE) were estimated for the least stabilized complexes and was found to be negligible (less than 0.05 kcal/mol) using counterpoise corrections. Natural Bonding Orbital (NBO) and Natural Population Analysis (NPA) were performed to analyse the bonding[10]. In the case of the NBO analysis, Wiberg bond indexes were determined.

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Cartesian coordinates of all optimized structures and associated energies

Yb ;
scf done: -1159,57180572

HgC6F5_2

23
scf done: -1608.598513

C	-0.000012	-0.000394	2.077332
Hg	-0.000023	-0.000854	0.000021
C	-0.000020	-0.000320	-2.077334
C	-1.186257	-0.000464	-2.798660
C	-1.208457	-0.000117	-4.189743
C	0.000008	0.000394	-4.883287
C	1.208459	0.000552	-4.189719
C	1.186232	0.000191	-2.798636
F	-2.362982	-0.000958	-2.149876
F	-2.359235	-0.000266	-4.861394
F	0.000022	0.000733	-6.212658
F	2.359251	0.001042	-4.861346
F	2.362944	0.000354	-2.149827
C	-0.000119	1.186009	2.798385
C	-0.000106	1.208530	4.189463
C	0.000017	0.000226	4.883287
C	0.000126	-1.208385	4.189996
C	0.000109	-1.186478	2.798908
F	-0.000238	2.362584	2.149327
F	-0.000208	2.359464	4.860846
F	0.000031	0.000519	6.212657
F	0.000244	-2.359023	4.861887
F	0.000214	-2.363340	2.150370

YbFC6F4-Hg-C6F5mnr-opt (adduit du TS1) ;

24
scf done: -2768,17193874

C	1.000366	-0.449395	-3.107217	0.374849
C	-0.198055	-0.386490	-2.408904	-0.401334
C	-1.366596	-0.275572	-3.150532	0.374759
C	-1.359826	-0.227552	-4.540889	0.281906
C	-0.140068	-0.292811	-5.211476	0.295989
C	1.050927	-0.404373	-4.496755	0.282045
Hg	-0.241446	-0.453518	-0.335081	60.525346
Yb	1.813563	4.481614	3.522702	27.946484
F	-2.552464	-0.211129	-2.522239	-0.298065
F	-2.492948	-0.120706	-5.233172	-0.289601
F	-0.112334	-0.248700	-6.539644	-0.285766
F	2.211716	-0.466469	-5.147299	-0.289529
F	2.159360	-0.557440	-2.436446	-0.297723
C	-0.285983	-0.520280	1.743779	-0.390701
C	-0.775969	-1.632353	2.415810	0.375930
C	-0.819413	-1.703748	3.805267	0.283229
C	-0.354719	-0.622882	4.551620	0.305471
C	0.143398	0.506164	3.906508	0.277203
C	0.168148	0.537137	2.518678	0.371542
F	-1.229035	-2.686582	1.718722	-0.295704
F	0.655840	1.646018	1.919446	-0.291928
F	0.589344	1.542168	4.632649	-0.284335

F	-0.386693	-0.669726	5.878673	-0.282908
F	-1.294814	-2.781789	4.425196	-0.287401

YbFC6F4-Hg-C6F5 (TS1) ;

24

scf done: -2768.170865

C	0.995510	-0.641011	-2.933592
C	-0.142316	-0.242439	-2.244594
C	-1.199257	0.261749	-2.991263
C	-1.141265	0.373244	-4.376826
C	0.015359	-0.035685	-5.037877
C	1.093770	-0.547016	-4.318356
Hg	-0.262146	-0.393478	-0.177142
Yb	2.137292	3.757416	1.931634
F	-2.323426	0.661355	-2.372725
F	-2.167084	0.860672	-5.073753
F	0.090200	0.062076	-6.361620
F	2.194848	-0.935802	-4.959991
F	2.045460	-1.138049	-2.258911
C	-0.382143	-0.544727	1.893201
C	-0.352569	-1.776734	2.533370
C	-0.404671	-1.895050	3.919032
C	-0.486586	-0.740575	4.694347
C	-0.518775	0.512031	4.085025
C	-0.473138	0.581800	2.698114
F	-0.265687	-2.903980	1.809061
F	-0.509497	1.813640	2.133615
F	-0.591499	1.615087	4.829751
F	-0.535217	-0.834895	6.019004
F	-0.374865	-3.088042	4.509892

YbFC6F4-Hg-C6F5mnf-opt (produit TS1) ;

24

scf done: -2768,17463298

C	1.079460	-0.539981	-2.787830	0.370191
C	0.002482	-0.009072	-2.091318	-0.386576
C	-1.020788	0.558692	-2.837585	0.372496
C	-0.986952	0.610116	-4.226995	0.277440
C	0.110140	0.070435	-4.895426	0.290639
C	1.153057	-0.510123	-4.176441	0.277280
Hg	-0.076168	-0.064844	-0.009956	60.475343
Yb	1.526494	3.013828	0.805208	28.049334
F	-2.088030	1.087653	-2.211831	-0.299790
F	-1.982425	1.161088	-4.922757	-0.293296
F	0.161740	0.109118	-6.224832	-0.290169
F	2.198011	-1.026590	-4.824208	-0.293014
F	2.097953	-1.101957	-2.113188	-0.298208
C	-0.325393	-0.399718	2.045023	-0.351442
C	-0.218429	-1.687300	2.557867	0.366569
C	-0.357932	-1.967114	3.913970	0.287551
C	-0.616958	-0.921899	4.797917	0.290164
C	-0.727278	0.383154	4.322925	0.289261
C	-0.585239	0.610629	2.959448	0.332719
F	0.033275	-2.715011	1.730862	-0.294209
F	-0.692251	1.898789	2.535818	-0.305877
F	-0.970610	1.382694	5.170246	-0.290647
F	-0.758035	-1.168815	6.096757	-0.286753
F	-0.253826	-3.212187	4.375720	-0.288884

C6F5-insertion-Yb-HgC6F5IRCrOPT (adduit TS2) ;

24
scf done: -2768.174638

C	1.487134	0.124022	-2.182240
C	0.210533	0.073370	-1.635638
Hg	-0.060745	0.194067	0.435527
C	-0.120368	0.112342	2.517468
C	0.641484	0.974816	3.293822
C	0.617966	0.940225	4.684077
C	-0.195948	0.006356	5.322089
C	-0.971024	-0.876306	4.572464
C	-0.916928	-0.808163	3.184326
C	1.715599	0.053262	-3.553006
C	0.628009	-0.076356	-4.414079
C	-0.666843	-0.128653	-3.902453
C	-0.846290	-0.057127	-2.525773
F	-1.675154	-1.667891	2.480104
F	1.430799	1.886116	2.698093
F	1.357820	1.780176	5.408790
F	-0.233136	-0.042963	6.651494
F	-1.745371	-1.768660	5.190901
Yb	-2.783358	2.503260	-0.064030
F	-2.116808	-0.100718	-2.061173
F	-1.705010	-0.248944	-4.730117
F	0.825530	-0.148988	-5.727299
F	2.950658	0.102433	-4.050697
F	2.553383	0.250487	-1.374830

C6F5-insertion-Yb-HgC6F5 (TS2) ;

24
scf done: -2768.165647

C	0.781375	0.210051	-1.626309
C	-0.554135	0.583830	-1.613783
Hg	-1.473551	1.282487	0.598902
C	-0.495931	0.506209	2.372393
C	0.364323	1.285920	3.124528
C	0.977710	0.815173	4.281945
C	0.713682	-0.486142	4.702258
C	-0.149160	-1.296310	3.968404
C	-0.737669	-0.781022	2.817085
C	1.430818	-0.271488	-2.761488
C	0.723258	-0.383615	-3.959129
C	-0.616676	-0.010317	-4.009612
C	-1.175248	0.447915	-2.825111
F	-1.569943	-1.588385	2.125601
F	0.639895	2.549667	2.741252
F	1.809403	1.584253	4.992380
F	1.288674	-0.957472	5.810460
F	-0.395733	-2.544776	4.379045
Yb	-3.229885	2.458214	-1.409252
F	-2.552002	0.831868	-2.944955
F	-1.306941	-0.097733	-5.151156
F	1.329973	-0.838683	-5.054860
F	2.716301	-0.629490	-2.734866
F	1.523393	0.306010	-0.505913

C6F5-insertion-Yb-HgC6F5IRCfOPT (produit TS2) ;

24
scf done: -2768.218908

C	0.997423	1.438291	-4.259894
C	-0.034681	1.016319	-3.437210
Hg	-0.698148	0.473399	1.609175
C	-0.298746	0.037635	3.762251
C	0.636527	0.751771	4.489631
C	0.903516	0.500554	5.832369
C	0.198714	-0.514648	6.475094
C	-0.752113	-1.256918	5.778306
C	-0.977301	-0.961308	4.437074
C	1.171579	0.952826	-5.555000
C	0.280488	0.003321	-6.061162
C	-0.777619	-0.457249	-5.279024
C	-0.865688	0.085486	-4.007437
F	-1.908076	-1.700863	3.789698
F	1.337770	1.745110	3.896033
F	1.813270	1.206641	6.513468
F	0.434396	-0.776468	7.762219
F	-1.422868	-2.228885	6.407512
Yb	-1.254854	1.033588	-1.331496
F	-1.943743	-0.375736	-3.193336
F	-1.634641	-1.362631	-5.754009
F	0.441542	-0.462256	-7.298130
F	2.171618	1.375467	-6.330599
F	1.883566	2.352718	-3.827712

C6F5-Yb-Hg-C6F5fopt (adduit TS3) ;

24
scf done: -2768.218922

C	-1.629799	1.296827	-4.165843
C	-1.796254	0.417243	-3.108088
C	-2.189563	-0.843400	-3.479338
C	-2.426641	-1.309379	-4.762276
C	-2.242242	-0.381534	-5.786278
C	-1.843770	0.924840	-5.492191
Yb	-1.737880	-0.133097	-0.738909
F	-2.374550	-1.780897	-2.418759
F	-2.808717	-2.558628	-5.032903
F	-2.448782	-0.741568	-7.051390
F	-1.679109	1.789141	-6.495169
F	-1.250537	2.567440	-3.942830
Hg	0.212131	0.014230	1.596378
C	1.616445	0.120637	3.329391
C	2.988964	0.064559	3.165375
C	3.881391	0.129096	4.231611
C	3.372819	0.255744	5.522340
C	1.996731	0.315651	5.730291
C	1.152138	0.246598	4.626323
F	3.516081	-0.058055	1.925515
F	-0.179586	0.307811	4.863432
F	1.520398	0.436808	6.974958
F	4.206491	0.319853	6.562419
F	5.205106	0.072824	4.045964

C6F5-Yb-Hg-C6F5 (TS3) ;

24
scf done: -2768.207541

C	1.444103	-0.345852	3.307287
C	0.548097	-0.398103	2.257607
C	-0.787187	-0.312878	2.592054
C	-1.258109	-0.182727	3.892640
C	-0.320032	-0.134707	4.921961
C	1.041738	-0.216087	4.634920
Hg	0.851501	-0.598996	-0.016643
Yb	-1.463026	-0.624717	-1.867415
F	-1.746654	-0.356606	1.597301
F	-2.564679	-0.103556	4.175434
F	-0.727829	-0.010288	6.186708
F	1.925164	-0.167727	5.637958
F	2.771312	-0.421550	3.069694
C	-2.343791	-0.078345	-4.055567
C	-2.911456	-1.314614	-4.232884
C	-3.617777	-1.767059	-5.335232
C	-3.762579	-0.852057	-6.377197
C	-3.214655	0.429038	-6.274269
C	-2.519501	0.790012	-5.121046
F	-2.750548	-2.236057	-3.155405
F	-4.137854	-2.991794	-5.424196
F	-4.427446	-1.200682	-7.476357
F	-3.373111	1.280633	-7.288629
F	-2.016116	2.035312	-5.075972

C6F5-Yb-Hg-C6F5IRCr (produit TS3) ;

24
scf done: -2768.260886

C	1.260615	0.700860	2.906110
C	0.370328	0.011835	2.102403
C	-0.779666	-0.379767	2.739833
C	-1.120582	-0.156262	4.064593
C	-0.185075	0.543152	4.825422
C	1.011857	0.975115	4.249540
Hg	2.839480	-0.066114	-0.923310
Yb	-0.283558	-0.937824	-0.062571
F	-1.719457	-1.091704	1.951183
F	-2.266233	-0.571748	4.610493
F	-0.432835	0.800016	6.109720
F	1.889228	1.640950	5.005266
F	2.436709	1.141335	2.405630
C	-0.934013	0.017559	-2.208814
C	-1.932121	-0.892027	-2.456318
C	-2.758872	-0.941156	-3.567906
C	-2.547055	0.043019	-4.532106
C	-1.546488	1.001088	-4.354671
C	-0.765251	0.967357	-3.201132
F	-2.131248	-1.890585	-1.471491
F	-3.711278	-1.862423	-3.735609
F	-3.299615	0.067028	-5.632092
F	-1.363048	1.926708	-5.300129
F	0.192842	1.910992	-3.087815

Hg ;
scf done: -153,613110139

YbC6F5_2

23
scf done: -2614.634684

C	-0.493252	0.387179	2.166868
Yb	-1.163209	0.953016	-0.086456
C	0.038826	0.654835	-2.175906
C	-0.925190	-0.158188	-2.715864
C	-0.915097	-0.761646	-3.963110
C	0.206181	-0.506601	-4.750943
C	1.232401	0.312043	-4.273749
C	1.129178	0.873608	-3.001920
F	-2.065683	-0.410340	-1.898246
F	-1.900773	-1.541779	-4.411761
F	0.298784	-1.044907	-5.966115
F	2.291649	0.538559	-5.054028
F	2.145877	1.655792	-2.597584
C	0.203317	1.244304	2.996380
C	0.605409	0.915321	4.286363
C	0.284034	-0.352451	4.771617
C	-0.421715	-1.256423	3.977523
C	-0.788563	-0.852466	2.698788
F	0.515990	2.488763	2.536605
F	1.278376	1.768944	5.065160
F	0.652074	-0.701823	6.004994
F	-0.724045	-2.465797	4.461177
F	-1.484570	-1.739945	1.930208

LH ;

15
scf done: -304.736589

C	0.037935	0.000000	-0.043704
C	0.047962	0.000000	1.371743
N	1.294698	0.000000	1.840676
N	2.066986	0.000000	0.738187
C	1.367495	0.000000	-0.425477
H	-0.821723	0.000000	-0.699054
C	2.021003	0.000000	-1.766477
H	1.261508	0.000000	-2.550946
H	2.651142	0.884855	-1.914421
H	2.651142	-0.884856	-1.914421
H	3.068263	0.000000	0.847528
C	-1.122456	0.000000	2.304451
H	-2.061907	-0.000001	1.746069
H	-1.112309	-0.881958	2.952968
H	-1.112310	0.881959	2.952967

YbC6F5_2-LIRCfopt (adduit TS1) ;

38
scf done: -2919.431651

C	-0.411373	2.270985	-1.878880
C	0.327979	1.150264	-2.171411
C	0.739425	1.086760	-3.485725
C	0.440457	2.045689	-4.448174
C	-0.327172	3.149983	-4.074782
C	-0.769053	3.282086	-2.759077
F	1.515185	0.034397	-3.900895
Yb	0.207798	0.215608	0.165873
C	-1.363720	-0.961531	1.657394
C	-2.305059	-1.947225	1.899910
C	-2.918316	-2.120670	3.139585
C	-2.580553	-1.273262	4.196466
C	-1.638293	-0.263591	4.011897
C	-1.084753	-0.170839	2.743820
F	-2.671473	-2.798373	0.920003
F	-3.824412	-3.082342	3.347592
F	-3.161009	-1.432425	5.387768
F	-1.308289	0.549974	5.020744
F	-0.122538	0.854156	2.553752
F	0.867008	1.941787	-5.710758
F	-0.629843	4.084551	-4.976579
F	-1.494475	4.342868	-2.396615
F	-0.839619	2.413211	-0.549001
N	2.771723	-1.106296	-1.433949
H	2.298386	-0.606568	-2.182581
N	2.254396	-1.080096	-0.184793
C	3.045783	-1.882370	0.546349
C	4.065048	-2.415496	-0.257627
C	3.855356	-1.898808	-1.530866
C	2.796881	-2.093238	2.004391
H	3.135444	-3.085514	2.312007
H	3.336000	-1.357930	2.612432
H	1.731472	-2.015148	2.240964
H	4.849677	-3.093153	0.045604
C	4.583804	-2.089531	-2.818298
H	5.608145	-1.710665	-2.747537
H	4.640395	-3.150467	-3.078672
H	4.083916	-1.564970	-3.636267

YbC6F5_2-L (TS1) ;

38
scf done: -2919.414742

C	0.237103	-0.270843	-2.359309
C	1.547435	-0.114926	-1.955294
C	2.150527	1.064177	-2.376552
C	1.491638	2.016745	-3.149779
C	0.164159	1.796223	-3.519196
C	-0.494692	0.638568	-3.109669
F	3.429826	1.313927	-2.050885
Yb	0.713183	-1.552267	0.253385
C	-0.842510	-1.665176	2.145014
C	-1.905730	-2.244058	2.816347
C	-2.373868	-1.770002	4.040671
C	-1.756063	-0.665702	4.630920
C	-0.680107	-0.042581	4.001345
C	-0.289039	-0.587401	2.788225
F	-2.541633	-3.313340	2.297158
F	-3.403213	-2.346373	4.669359
F	-2.197578	-0.205693	5.802560
F	-0.084257	1.014480	4.560930
F	0.806364	0.037354	2.136624
F	2.101598	3.132675	-3.545816
F	-0.478837	2.700250	-4.251223
F	-1.768297	0.432835	-3.439595
F	-0.441114	-1.408567	-1.922989
N	3.108132	-2.140427	-1.062246
H	2.386723	-1.126946	-1.520161
N	2.501354	-2.990559	-0.176283
C	3.342193	-4.017007	0.040520
C	4.501251	-3.830818	-0.719895
C	4.311256	-2.629530	-1.406632
C	2.990059	-5.122605	0.982407
H	3.021220	-6.095425	0.480951
H	3.688921	-5.167449	1.824477
H	1.983571	-4.983351	1.386122
H	5.366792	-4.477237	-0.765026
C	5.193656	-1.927472	-2.387291
H	6.244707	-2.026333	-2.102797
H	5.084901	-2.348233	-3.393609
H	4.952052	-0.863316	-2.438773

YbC6F5_2-LIRCropt (produit TS1) ;

38
scf done: -2919.443025

C	-0.009620	1.002640	-2.465761
C	1.276775	0.630043	-2.808837
C	1.714336	0.949100	-4.087695
C	0.888323	1.616328	-4.991364
C	-0.402954	1.973677	-4.610118
C	-0.866875	1.665892	-3.332430
F	2.943664	0.619333	-4.476903
Yb	0.145937	-0.641920	0.766128
C	-1.169605	-0.777259	2.851173
C	-1.914364	-1.498387	3.768379
C	-2.464345	-0.927223	4.914777
C	-2.266136	0.431554	5.165914
C	-1.525331	1.207900	4.277273
C	-1.019068	0.550107	3.166501
F	-2.142788	-2.814472	3.580060
F	-3.181213	-1.647288	5.784768
F	-2.789057	0.988793	6.260303
F	-1.332889	2.510511	4.512164
F	-0.265489	1.335881	2.261664
F	1.321087	1.914162	-6.212059
F	-1.196358	2.608872	-5.464473
F	-2.098278	2.003152	-2.961318
F	-0.495130	0.718508	-1.215741
N	2.314163	-1.025972	0.067289
H	1.921109	0.107650	-2.106758
N	1.521082	-2.009955	-0.498409
C	2.308062	-2.818320	-1.224512
C	3.630535	-2.364211	-1.145303
C	3.585965	-1.238895	-0.314948
C	1.750215	-3.998290	-1.954367
H	2.036248	-3.988554	-3.011423
H	2.114369	-4.939813	-1.528271
H	0.658681	-4.003445	-1.895113
H	4.502530	-2.796431	-1.617935
C	4.698673	-0.359371	0.159883
H	5.315046	-0.866488	0.911045
H	5.360873	-0.071658	-0.662860
H	4.300944	0.551311	0.615727

YbC6F5-L2IRCfopt (adduit TS2) ;

41
scf done: -2496.104932

N	-1.741017	0.933280	-0.760882
N	-2.354784	-0.047577	-1.459507
C	-3.514553	0.356997	-2.012620
C	-3.668017	1.687678	-1.646270
C	-2.540905	2.005482	-0.868510
Yb	0.441856	0.430843	0.251028
F	-1.273280	-2.783570	-2.061526
C	-0.414919	-3.075181	-1.030078
C	-0.163563	-4.425378	-0.807924
C	0.686636	-4.781268	0.239711
C	1.255871	-3.794565	1.043201
C	0.935595	-2.479239	0.737342
C	0.118526	-2.049312	-0.280083
F	-0.710291	-5.385523	-1.562608
F	0.948182	-6.068509	0.476972
F	2.063546	-4.134504	2.052461
F	1.498895	-1.490829	1.557595
C	-4.369481	-0.562086	-2.818746
C	-2.187431	3.301529	-0.215583
N	1.270475	2.361640	1.262969
N	1.909554	2.198590	0.047874
C	2.806275	3.186805	-0.093656
C	2.760483	4.012753	1.034925
C	1.780516	3.450451	1.860662
C	3.671673	3.282072	-1.309846
C	1.301068	3.892924	3.206857
H	-1.911500	-0.959528	-1.534576
H	-2.946719	3.589118	0.519247
H	-1.222402	3.237487	0.295116
H	-2.126413	4.106536	-0.954764
H	-4.487422	2.340928	-1.908763
H	-4.686335	-0.080791	-3.747889
H	-3.831734	-1.478470	-3.074806
H	-5.272225	-0.844440	-2.266851
H	4.730702	3.145988	-1.062484
H	3.393940	2.512979	-2.035634
H	3.575466	4.258866	-1.796405
H	0.500192	3.237303	3.559464
H	2.107292	3.868658	3.948652
H	0.915477	4.918316	3.181979
H	3.357615	4.894146	1.228776

YbC6F5-L2 (TS2) ;

41
scf done: -2496.090316

N	1.514511	1.764125	-1.124361
N	1.319902	0.549239	-1.720290
C	0.173906	0.566734	-2.420691
C	-0.399461	1.832638	-2.280198
C	0.477173	2.550665	-1.459731
Yb	3.656790	1.283922	-0.264104
F	3.168574	-1.994976	-3.434258
C	3.544741	-2.222419	-2.164258
C	4.255382	-3.392613	-1.910333
C	4.657247	-3.676440	-0.604851
C	4.356551	-2.791806	0.428383
C	3.628973	-1.656546	0.098582
C	3.205438	-1.313499	-1.169390
F	4.557766	-4.248606	-2.886457
F	5.342401	-4.787462	-0.348724
F	4.756038	-3.047206	1.673860
F	3.367681	-0.764507	1.133600
C	-0.310774	-0.634829	-3.166127
C	0.388406	3.963928	-0.980873
N	5.128817	2.733193	0.738149
N	5.594364	2.478326	-0.540130
C	6.724637	3.177429	-0.723281
C	7.009825	3.899815	0.440751
C	5.976644	3.587635	1.331151
C	7.479606	3.110385	-2.012495
C	5.748037	4.064717	2.730006
H	2.231660	-0.394903	-1.477175
H	-0.537699	4.138270	-0.422886
H	1.229050	4.203945	-0.324049
H	0.402840	4.670928	-1.817352
H	-1.323548	2.182558	-2.719493
H	-0.886375	-0.336905	-4.046416
H	0.527091	-1.252678	-3.498955
H	-0.961937	-1.258564	-2.542432
H	8.475796	2.675280	-1.873505
H	6.940707	2.495218	-2.737960
H	7.618310	4.105832	-2.448024
H	4.853353	3.597845	3.150566
H	6.595104	3.821207	3.380685
H	5.612377	5.151424	2.767216
H	7.850088	4.558886	0.614904

YbC6F5-L2IRCropt (produit TS2) ;

41
scf done: -2496.115900

N	-1.820408	1.243776	-0.463170
N	-1.303799	0.919424	-1.703404
C	-2.333144	0.699178	-2.540898
C	-3.536036	0.870025	-1.845393
C	-3.160057	1.219671	-0.542759
Yb	0.493486	1.324404	-0.241288
F	-3.176587	-3.471514	-1.050327
C	-2.025590	-3.400197	-0.384817
C	-1.618985	-4.508363	0.356961
C	-0.418502	-4.461842	1.061626
C	0.371323	-3.314116	1.026541
C	-0.071440	-2.235084	0.273652
C	-1.257706	-2.244349	-0.436419
F	-2.364959	-5.608414	0.397777
F	-0.023218	-5.513210	1.771211
F	1.518454	-3.264091	1.697851
F	0.727041	-1.123943	0.256252
C	-2.104731	0.356703	-3.979273
C	-4.014780	1.541911	0.641480
N	1.936384	2.631121	1.029637
N	2.234471	2.842720	-0.304450
C	3.222607	3.747861	-0.376885
C	3.583942	4.137176	0.917561
C	2.744550	3.407790	1.767236
C	3.770565	4.194826	-1.694896
C	2.667164	3.409686	3.260976
H	-1.573932	-1.379622	-1.014703
H	-4.724927	0.736233	0.857285
H	-3.393548	1.696333	1.527726
H	-4.599651	2.453955	0.477277
H	-4.540480	0.764590	-2.233726
H	-2.375666	1.190562	-4.637207
H	-1.050610	0.124350	-4.153908
H	-2.703136	-0.506808	-4.287997
H	4.839942	3.972433	-1.784085
H	3.250142	3.689976	-2.513274
H	3.651665	5.275157	-1.834264
H	1.893968	2.715696	3.601679
H	3.617863	3.107597	3.714655
H	2.424115	4.404663	3.650501
H	4.346797	4.850661	1.200397

YbL2 ;

29
scf done: -1767.993666

C	0.960760	0.596236	-0.294671
C	-0.210296	-0.146402	-0.108486
C	-0.001550	-0.870747	1.070371
N	1.214525	-0.580693	1.557839
N	1.814153	0.333577	0.707094
C	-0.907571	-1.835200	1.767594
C	1.317760	1.552444	-1.387961
H	-1.088809	-0.157886	-0.740084
H	0.601864	2.379644	-1.448435
H	2.310518	1.976365	-1.214281
H	1.326710	1.059732	-2.366704
Yb	3.309226	-0.089940	2.422064
H	-1.161785	-2.685180	1.124568
H	-0.427526	-2.225052	2.669266
H	-1.849451	-1.360116	2.063854
N	5.399301	-0.469593	3.352077
N	4.808624	0.563463	4.061559
C	5.664232	0.958612	5.016808
C	6.827667	0.185056	4.941491
C	6.612151	-0.698808	3.878381
C	7.508752	-1.762235	3.328416
H	7.023246	-2.276265	2.494415
H	8.453338	-1.343161	2.963992
H	7.758467	-2.510851	4.088527
H	7.705461	0.255472	5.570265
C	5.317648	2.067943	5.958325
H	6.021875	2.903100	5.872922
H	4.314998	2.448610	5.745658
H	5.338539	1.731875	7.000967

HC6F5

12
scf done: -727.958130

C	-0.082569	0.107328	-0.046268
C	-0.128724	-0.230019	1.340361
C	1.021075	0.084859	2.045628
C	2.194435	0.251947	1.266498
C	2.280568	0.088570	-0.139811
C	1.094584	-0.226172	-0.782182
F	-1.140046	-0.827395	1.952313
F	1.163289	-0.032705	3.372198
F	3.325210	0.461486	1.918494
F	3.499843	-0.025822	-0.681992
F	1.118234	-0.819943	-1.965907
H	0.203329	1.167863	0.120667