Electronic supporting information

Steric Control in Metal-Ligand Electron Transfer of Iminopyridine-Ytterbocene Complexes

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Figure S13. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb^{2+}$[2,6-^{i}Pr$_2$C$_6$H$_3$NCH(C$_5$H$_3$N-C$_6$H$_5$)] (**3d**).

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Figure S16. IR spectrum of $(C_5Me_5)_2Yb^{2+}$[2,6-^{i}Pr$_2$C$_6$H$_3$NCH(C$_5$H$_3$N-C$_6$H$_5$)] (**3d**) (KBr, Nujol).

Figure S17. Thermal dependence of the susceptibility of **3d** on first (full circles) and second (empty triangles) heating.

Figure S18. Thermal dependence of the magnetic moment of **3d** on first (black and white circles) and second (full triangles) heating, the latter rescaled of a factor 2.05 to evidence the superimposability of the magnetic behaviour in the low temperature region.

Cartesian coordinates

Table S1. Crystallographic data and structure refinement details **3a–d**.

Compound	**3a**	**3b**	**3c**	**3d**
Empirical formula	$C_{38}H_{52}N_2Yb$	$C_{49}H_{62}N_2OYb$	$C_{42}H_{54}N_2SYb$	$C_{44}H_{56}N_2Yb$
Formula weight	709.85	868.04	791.97	785.94
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic
Space group	$P2_1/c$	$P2_1/c$	$Pna2_1$	$Pbca$
a, Å	14.9338(12)	12.0399(7)	16.0426(2)	17.8249(10)
b, Å	12.7510(9)	14.7771(8)	18.6629(3)	17.7694(10)
c, Å	17.6244(13)	24.3929(14)	12.4388(2)	23.7557(13)
α, °	90	90	90	90
β, °	98.707(2)	98.6090(10)	90	90
γ, °	90	90	90	90
V, Å^3	3317.4(4)	4291.0(4)	3724.20(10)	7524.3(7)
Z	4	4	4	8
d_{calc}, Mg/m^3	1.421	1.344	1.412	1.388
Absorption coefficient, mm^{-1}	2.847	2.216	2.598	2.518
F(000)	1456	1792	1624	3232
Crystal size, mm	0.60 × 0.28 × 0.26	0.15 × 0.14 × 0.13	0.50 × 0.30 × 0.05	0.32 × 0.17 × 0.08
θ range for data collection, °	2.51–29.00	2.18–28.70	3.01–31.00	2.06–26.02
Index ranges	–20 ≤ h ≤ 20 –17 ≤ k ≤ 17 –24 ≤ l ≤ 24	–16 ≤ h ≤ 16 –19 ≤ k ≤ 19 –32 ≤ l ≤ 32	–22 ≤ h ≤ 23 –26 ≤ k ≤ 27 –18 ≤ l ≤ 18	–21 ≤ h ≤ 22 –21 ≤ k ≤ 21 –29 ≤ l ≤ 29
Reflections collected	42132	44438	78244	61940
Independent reflections	8805	11078	11824	7412
R_{int}	0.0341	0.0561	0.0484	0.0905
Completeness to θ, %	99.7	99.9	99.8	100.0
Data / restraints / parameters	8805 / 0 / 388	11078 / 0 / 496	11824 / 1 / 434	7412 / 7 / 455
GooF on F^2	1.034	1.026	1.031	1.000
Final R indices ($I > 2\sigma(I)$)	R_1 = 0.0270 R_2 = 0.0649	R_1 = 0.0336 R_2 = 0.0727	R_1 = 0.0308 R_2 = 0.0600	R_1 = 0.0311 R_2 = 0.0605
R indices (all data)	R_1 = 0.0326 R_2 = 0.0667	R_1 = 0.0531 R_2 = 0.0800	R_1 = 0.0445 R_2 = 0.0644	R_1 = 0.0649 R_2 = 0.0690
Largest diff. peak and hole, e/Å^3	3.767 / –1.009	2.436 / –0.012	1.412 / –0.841	1.682 / –0.495

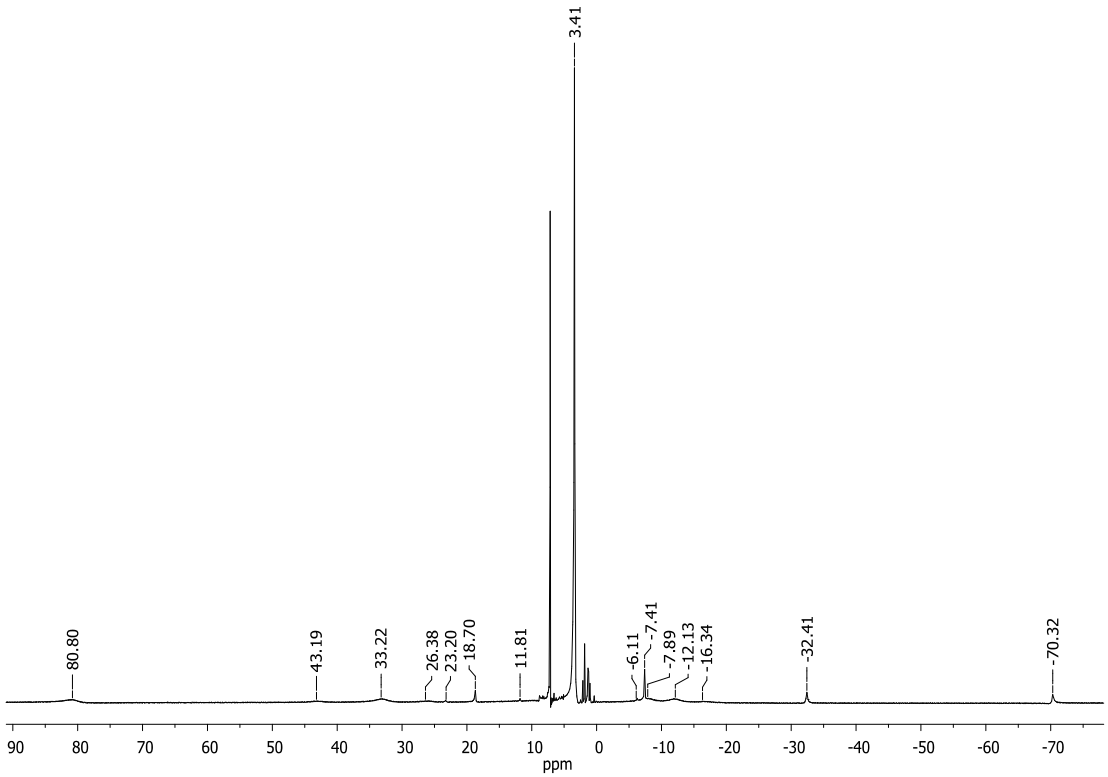


Figure S1. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb[2,6\text{-}^iPr_2(C_6H_3)NCH(C_5H_4N)]^{-\bullet}$ (**3a**) (200 MHz, C_6D_6, 293 K).

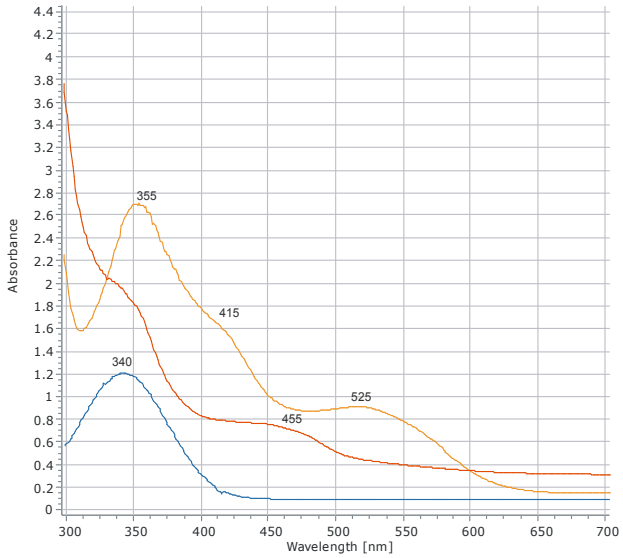


Figure S2. UV-vis spectra of $(C_5Me_5)_2Yb[2,6\text{-}^iPr_2(C_6H_3)NCH(C_5H_4N)]^{-\bullet}$ (**3a**) in nonane (red), radical-anionic adduct $[2,6\text{-}^iPr_2(C_6H_3)NCH(C_5H_4N)]^{-\bullet}K^+$ in THF (orange) and neutral **2a** in nonane (blue).

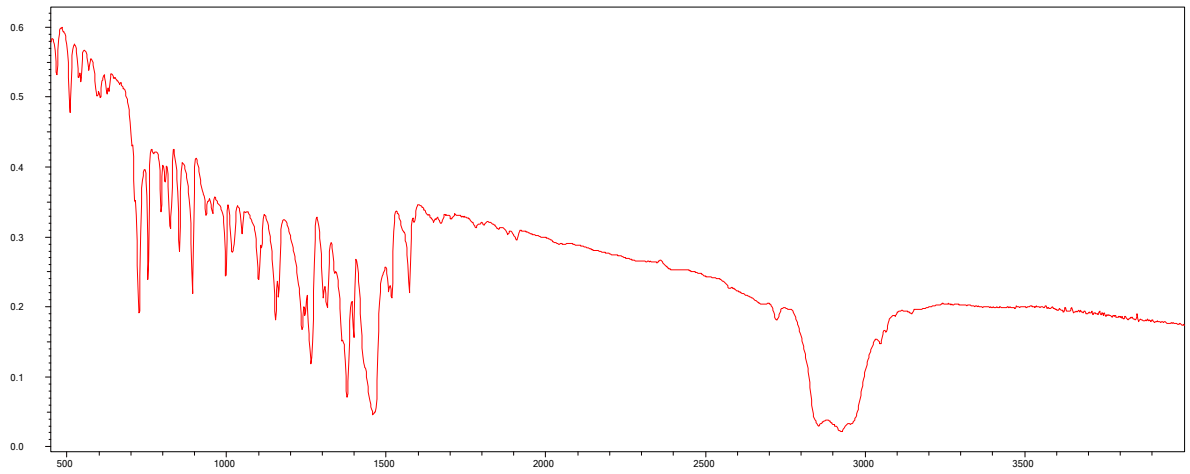


Figure S3. IR spectrum of $(C_5Me_5)_2Yb[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_4N)]^{-\cdot}$ (**3a**) (KBr, Nujol).

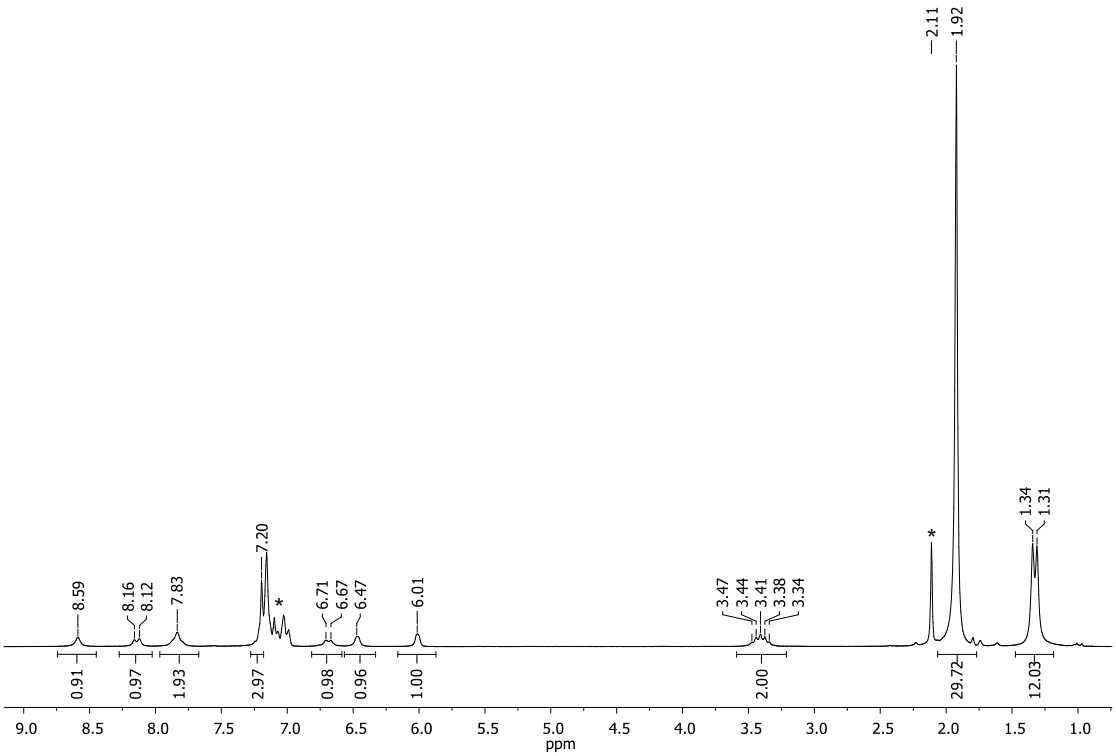


Figure S4. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3O)]$ (**3b**) (200 MHz, C_6D_6, 293 K); * - signals of toluene solvate.

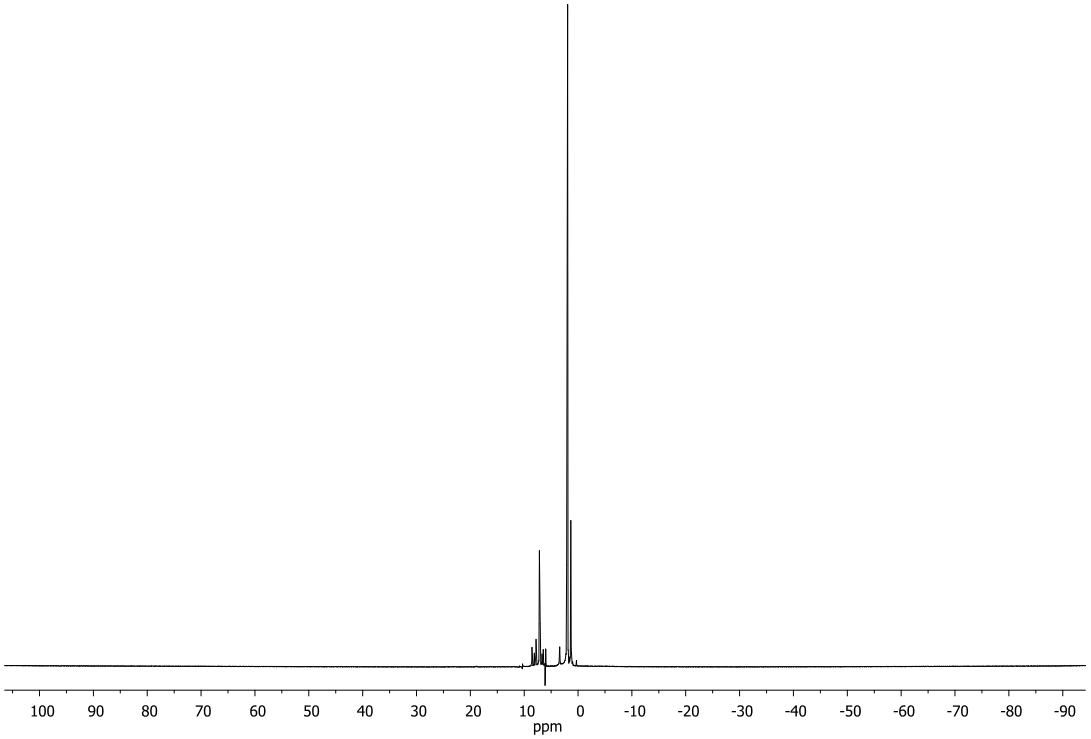


Figure S5. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3O)]$ (**3b**) (200 MHz, C_6D_6, 293 K), spectrum width – 200 ppm.

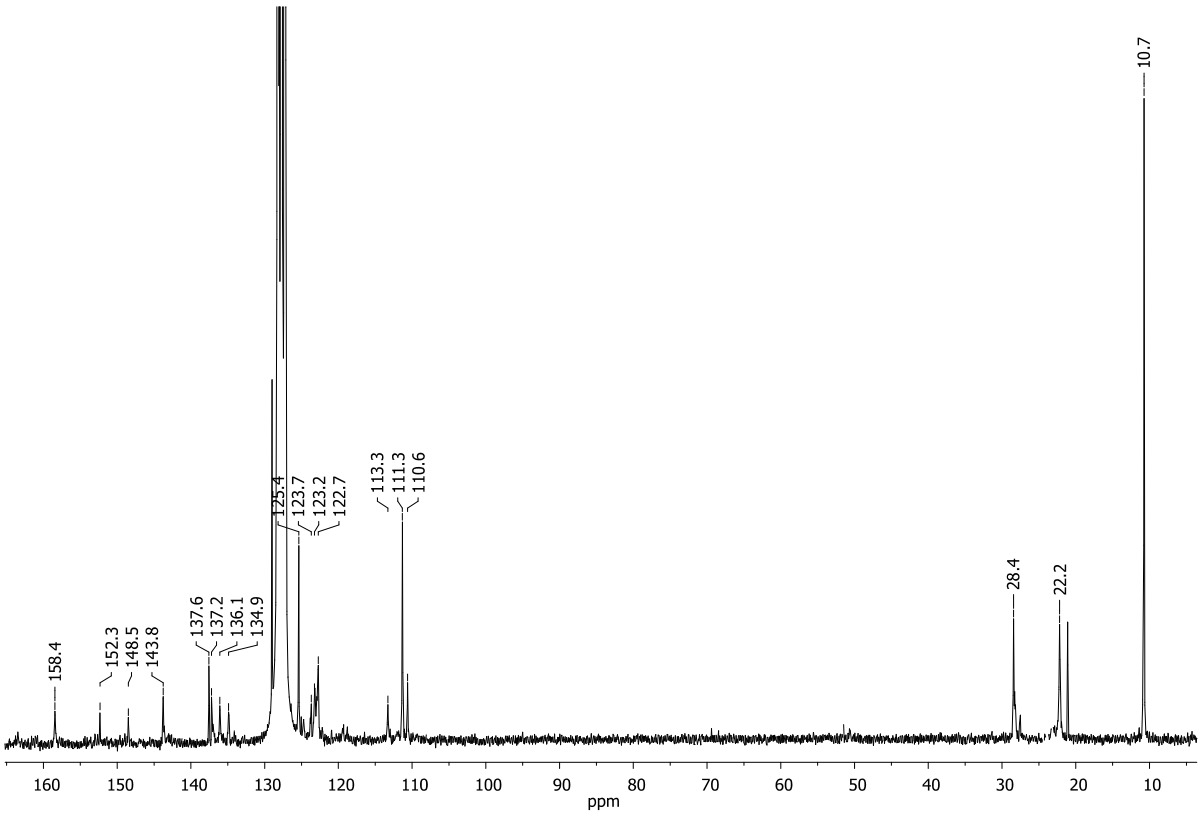


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3O)]$ (**3b**) (50 MHz, C_6D_6, 293 K).

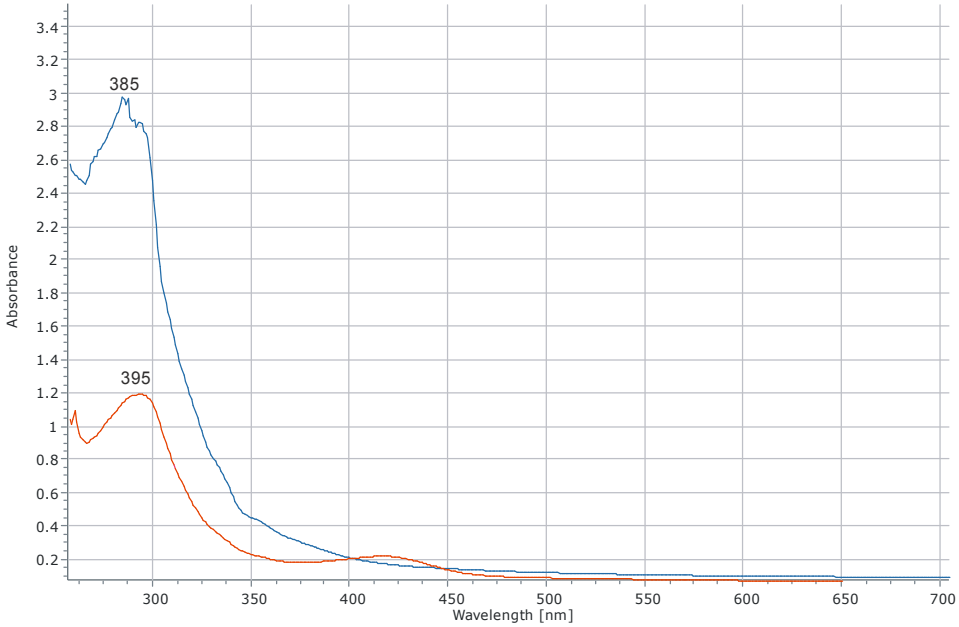


Figure S7. UV-Vis spectra of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3O)]$ (**3b**) – blue; neutral **2b** – red.

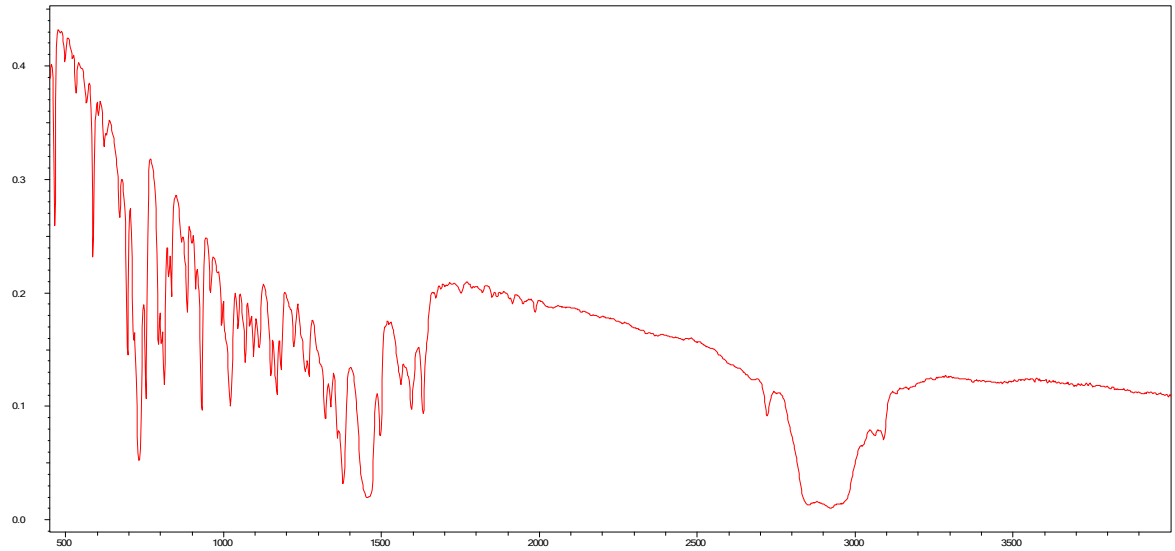


Figure S8. IR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3O)]$ (**3b**) (KBr, Nujol).

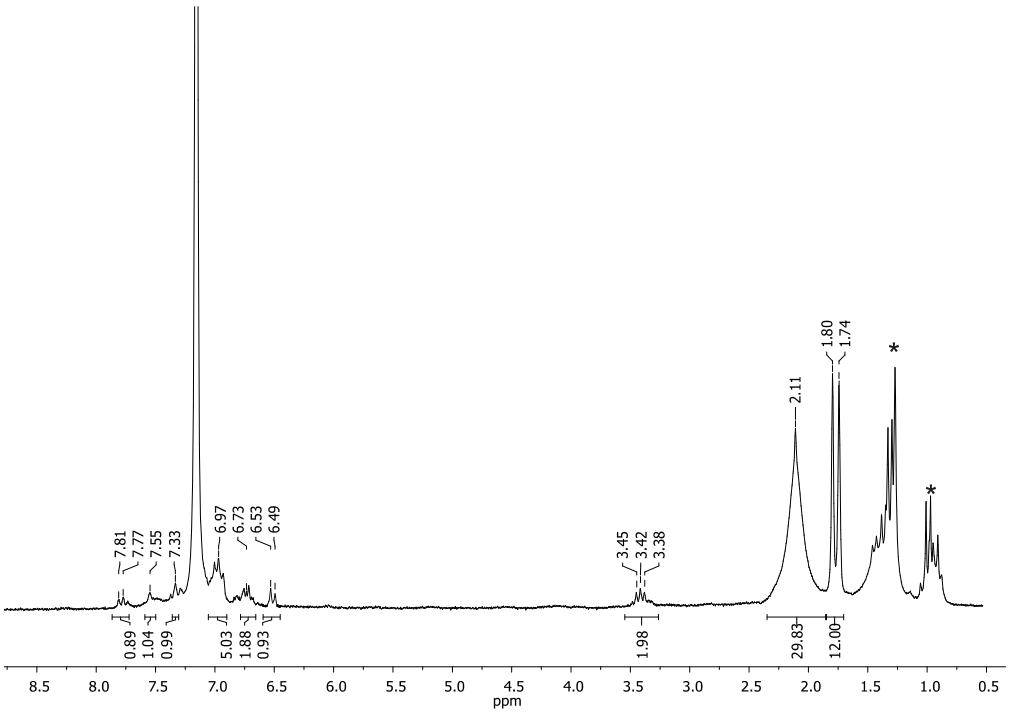


Figure S9. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3S)]$ (**3c**) (200 MHz, C_6D_6, 293 K); * – signals of nonane solvate.

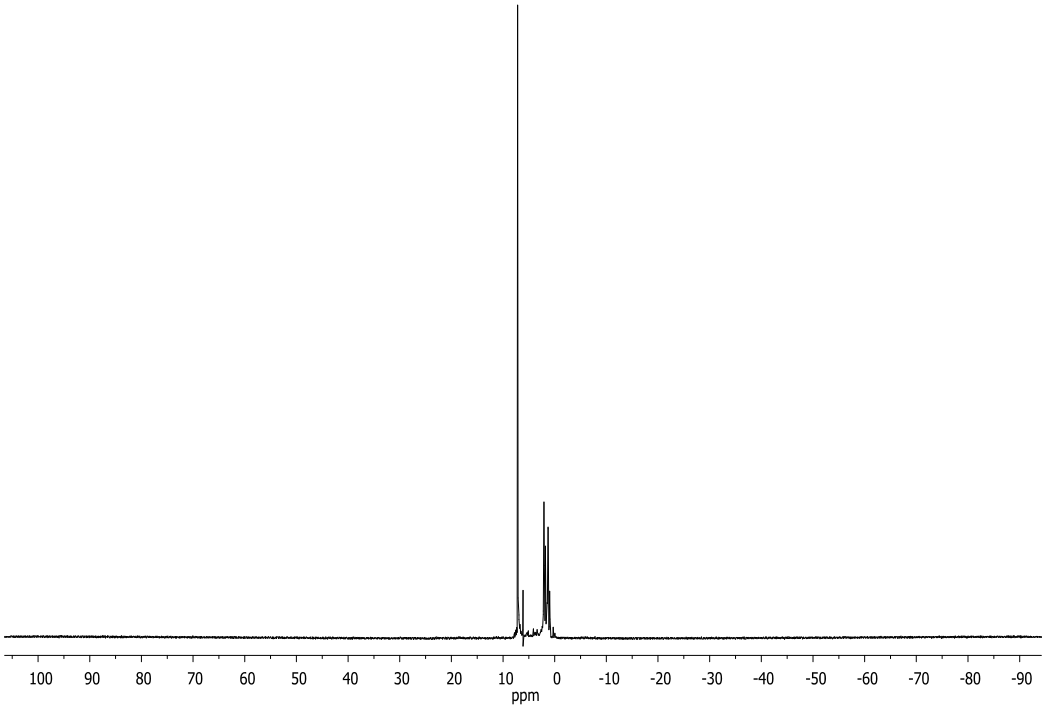


Figure S10. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3S)]$ (**3c**) (200 MHz, C_6D_6, 293 K); spectrum width – 200 ppm.

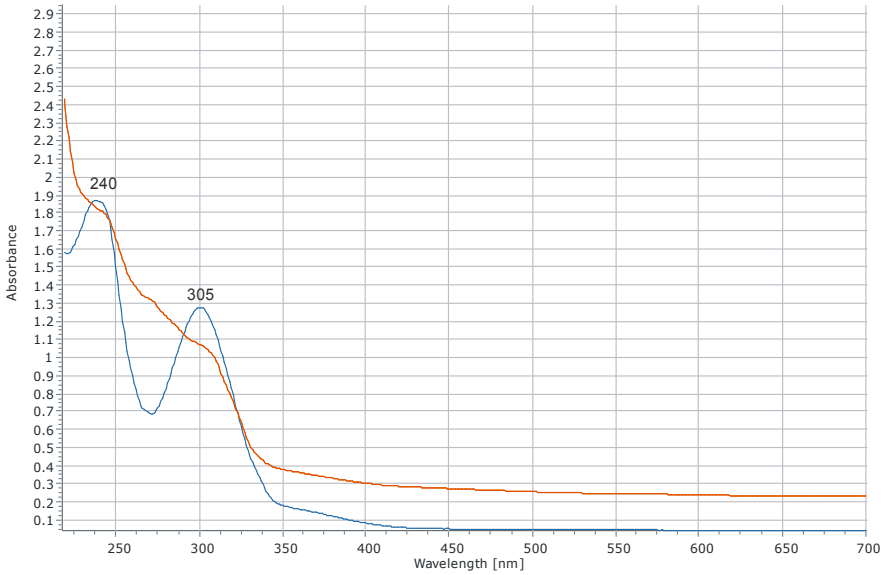


Figure S11. UV-Vis spectra of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3S)]$ (**3c**)– red; neutral **2c** – blue.

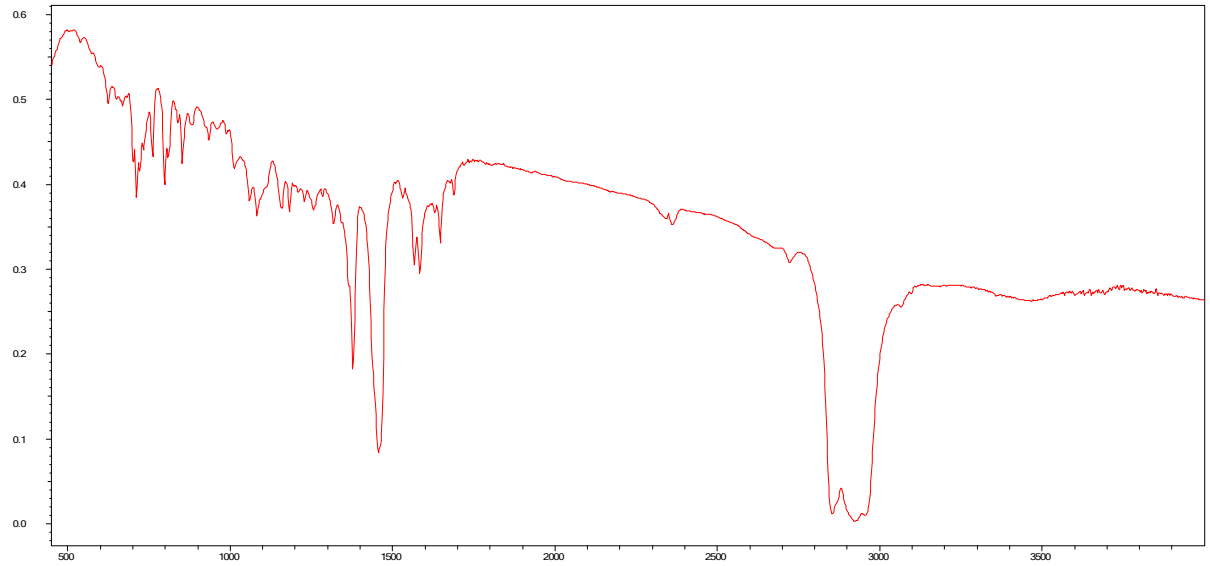


Figure S12. IR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_4H_3S)]$ (**3c**) (KBr, Nujol).

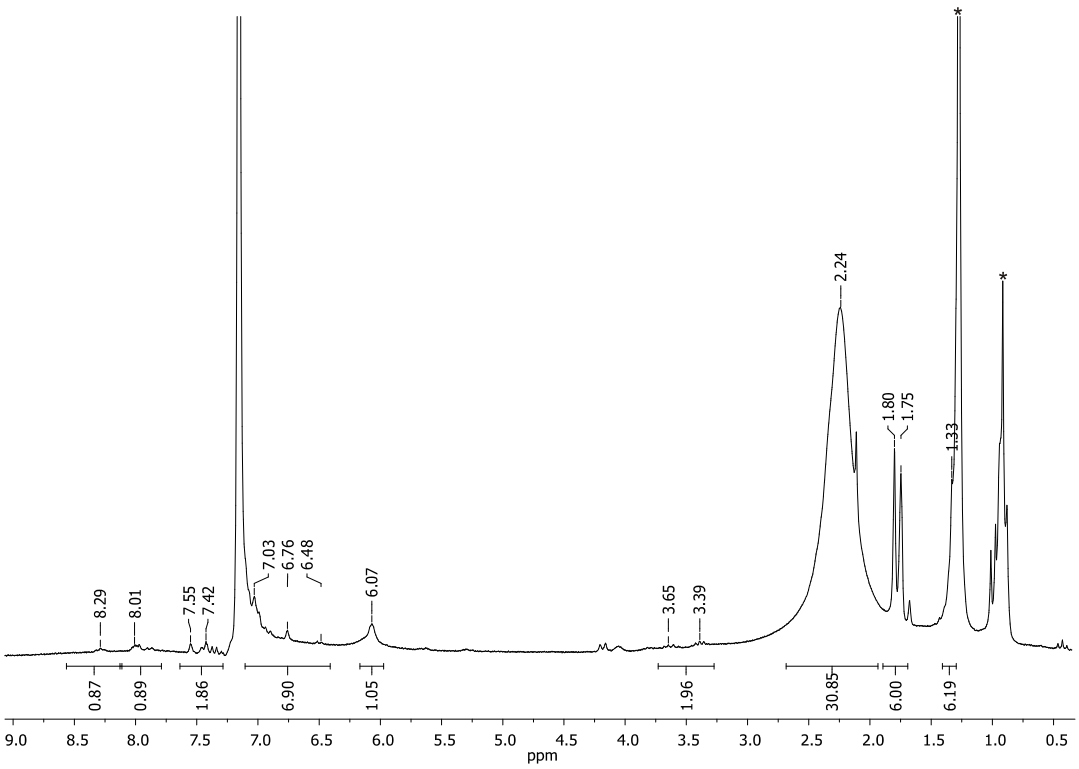


Figure S13. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^iPr_2C_6H_3NCH(C_5H_3N\text{-}C_6H_5)]$ (**3d**) (200 MHz, C_6D_6, 293 K); * – signals of nonane solvate.

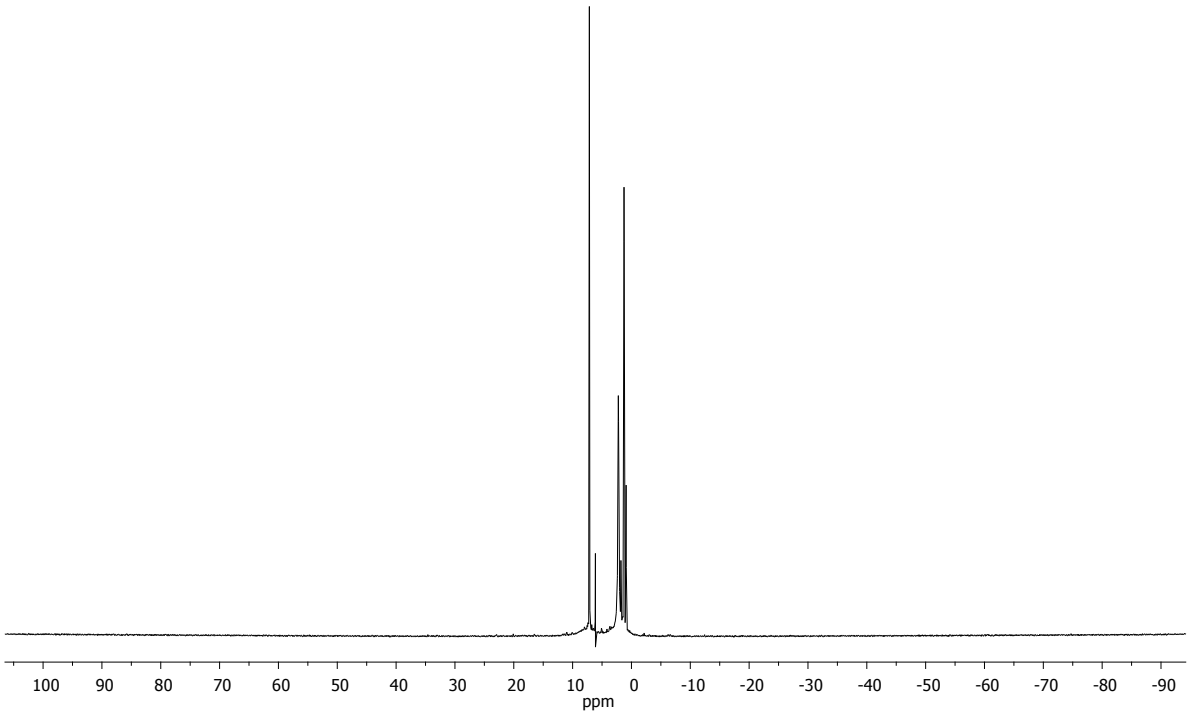


Figure S14. ^{1}H NMR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^iPr_2C_6H_3NCH(C_5H_3N\text{-}C_6H_5)]$ (**3d**) (200 MHz, C_6D_6, 293 K); spectrum width – 200 ppm.

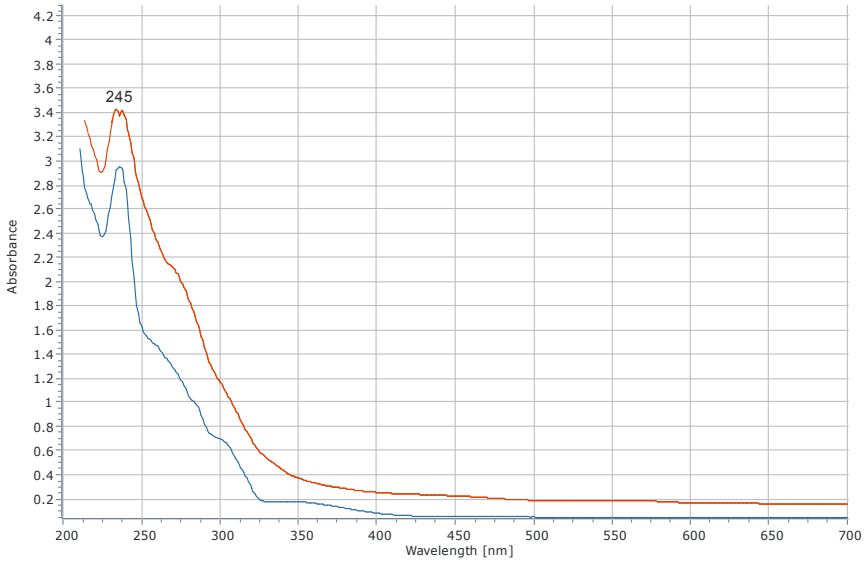


Figure S15. UV-Vis spectra of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_6H_5)]$ (**3d**) – red; neutral **2d** – blue.

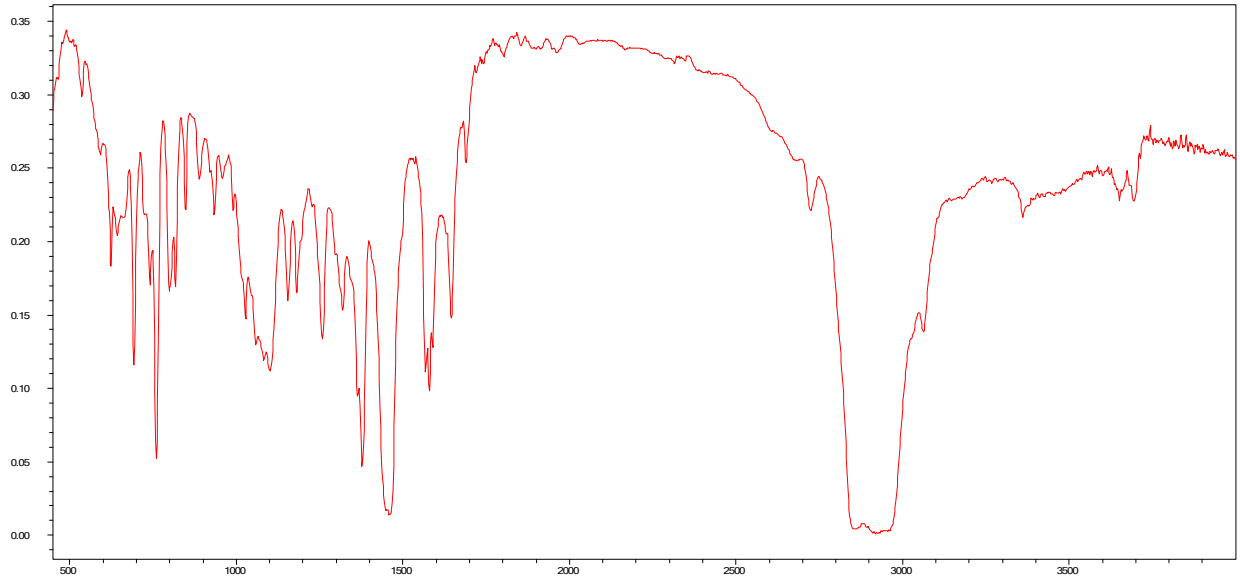


Figure S16. IR spectrum of $(C_5Me_5)_2Yb^{2+}[2,6\text{-}^{i}Pr_2C_6H_3NCH(C_5H_3N\text{-}C_6H_5)]$ (**3d**) (KBr, Nujol).

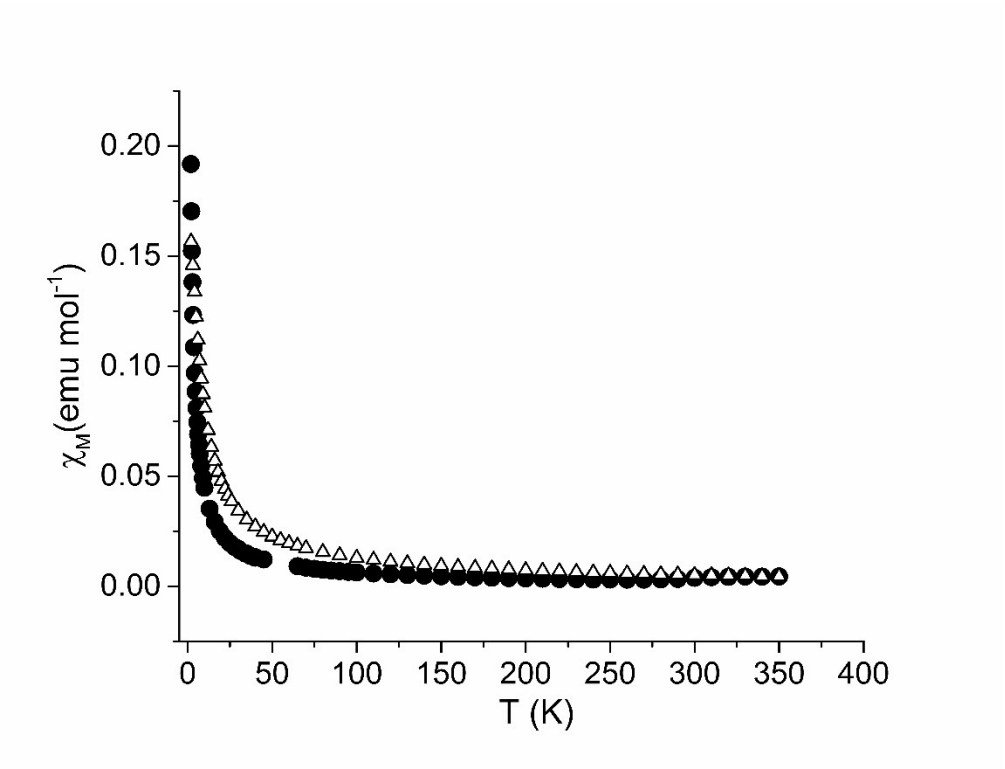


Figure S17. Thermal dependence of the susceptibility of **3d** on first (full circles) and second (empty triangles) heating.

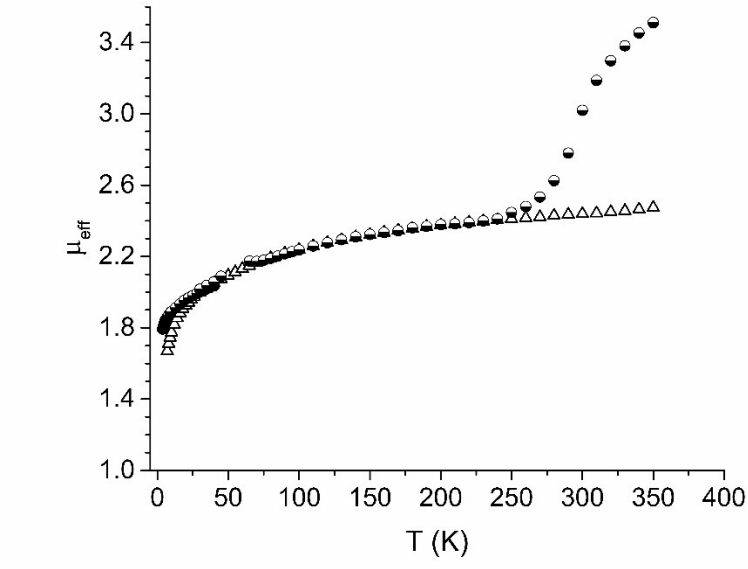


Figure S18. Thermal dependence of the magnetic moment of **3d** on first (black and white circles) and second (full triangles) heating, the latter rescaled of a factor 2.05 to evidence the superimposability of the magnetic behaviour in the low temperature region.

Cartesian coordinates

Yb(bisindenyl)
E = -1853.791562
H = -1853.515184
G = -1853.579497

Yb	-0.279241	1.883771	0.592592
C	0.925065	4.088182	-0.129616
C	0.854330	4.181673	1.295038
C	1.726201	3.203850	1.828025
C	2.313996	2.458453	0.779572
C	1.841110	3.006245	-0.453803
C	2.035105	2.641006	-1.810966
C	1.351858	3.319829	-2.804107
C	0.456093	4.374317	-2.487481
C	0.238788	4.757066	-1.175886
C	-2.477604	0.465254	0.583967
C	-2.781163	1.562244	1.449703
C	-2.000896	1.408295	2.619203
C	-1.173779	0.267132	2.500919
C	-1.468737	-0.347605	1.244611
C	-0.917611	-1.463597	0.563480
C	-1.352127	-1.764527	-0.715047
C	-2.338614	-0.972674	-1.358857
C	-2.895948	0.125443	-0.728461
H	-0.442761	5.573593	-0.946748
H	-0.060884	4.890810	-3.291806
H	1.503919	3.047199	-3.844972
H	2.724467	1.839335	-2.067644
H	1.915858	3.048693	2.885037
H	0.296127	4.917949	1.861835
H	3.051764	1.671539	0.889595
H	-0.938217	-2.623589	-1.236230
H	-2.661901	-1.239261	-2.361486
H	-3.656973	0.719585	-1.230076
H	-0.167556	-2.083795	1.049806
H	-0.497549	-0.113515	3.257704
H	-2.033056	2.067425	3.480514
H	-3.532430	2.324924	1.277847

THF
E = -232.380813
H = -232.257719
G = -232.292888

C	1.374144	-0.031742	-0.456380
O	0.158007	0.496670	0.053248
C	0.052352	0.000495	1.378405
C	1.466341	0.112883	1.964665
C	2.375004	-0.007281	0.717028
H	3.051960	0.848472	0.641842
H	2.990042	-0.912160	0.735627

H	1.600346	1.085413	2.447621
H	1.666175	-0.660670	2.712273
H	-0.699068	0.597954	1.901153
H	-0.284159	-1.050301	1.362574
H	1.212972	-1.063322	-0.810458
H	1.672247	0.583589	-1.309260

Yb(bisindenyl)(THF)2
E = -2318.584994
H = -2318.058288
G = -2318.152599

Yb	0.979981	1.664167	0.725353
C	0.672998	5.374872	-0.103176
C	1.254281	4.497267	0.845468
C	0.832297	4.027262	2.124880
C	1.891581	3.267378	2.668723
C	2.952214	3.182417	1.737136
C	2.587151	3.971106	0.605844
C	3.281120	4.348325	-0.570300
C	2.688983	5.219205	-1.467376
C	1.385193	5.731977	-1.235662
C	2.199172	-0.797796	1.186788
C	3.583412	-0.947976	0.913432
C	4.509865	-0.666229	1.899590
C	4.098170	-0.222750	3.183146
C	2.760049	-0.053181	3.480252
C	1.781373	-0.332511	2.494906
C	0.353673	-0.296364	2.507039
C	-0.090400	-0.777852	1.253085
C	1.018742	-1.052268	0.423396
O	1.442383	1.573860	-1.718349
C	0.841614	2.371066	-2.766686
C	1.800577	2.302801	-3.952187
C	2.519966	0.970466	-3.724028
C	2.645555	0.943487	-2.208274
O	-1.477273	2.147425	0.428040
C	-2.373412	1.983030	1.551933
C	-3.733877	2.476088	1.072222
C	-3.345016	3.547010	0.050119
C	-2.120382	2.922551	-0.605742
H	2.455636	0.272356	4.472913
H	4.849555	-0.020776	3.942338
H	5.569834	-0.799415	1.697563
H	3.914742	-1.324270	-0.052851
H	-1.126290	-0.923364	0.962878
H	-0.267255	-0.057812	3.363537
H	0.973512	-1.471808	-0.575377
H	0.955316	6.435099	-1.945406
H	3.236477	5.540200	-2.350673
H	4.294339	3.989017	-0.741655
H	-0.307421	5.810009	0.085355
H	-0.085168	4.300555	2.633927
H	1.891419	2.804590	3.649370

H	3.897934	2.677693	1.895949
H	-1.990240	2.585353	2.384408
H	-2.363056	0.930812	1.844678
H	-2.404639	2.244384	-1.421773
H	-1.400246	3.655720	-0.978240
H	-3.073678	4.480645	0.555161
H	-4.136121	3.766490	-0.672267
H	1.907626	0.130976	-4.072772
H	3.491965	0.915285	-4.222019
H	1.275962	2.353197	-4.910469
H	2.512540	3.133203	-3.906488
H	-0.132396	1.925258	-3.004361
H	0.704858	3.388951	-2.390959
H	2.691125	-0.058844	-1.778667
H	3.512252	1.521809	-1.863668
H	-4.345234	2.861880	1.892561
H	-4.288943	1.665354	0.586660

N2Ph (2a in *Dalton Trans., 2011,40,10568*)
E = -1039.375785
H = -1038.909512
G = -1038.992497

C	-2.797862	1.545883	0.834138
C	-2.077716	0.347763	1.052234
C	-2.624509	-0.909541	0.691201
C	-3.862058	-0.914039	0.032566
C	-4.545614	0.260864	-0.258971
C	-4.012804	1.482043	0.150248
N	-0.838013	0.455055	1.722834
C	0.223871	0.096601	1.116386
C	1.567256	0.154951	1.726577
C	2.660510	-0.309577	0.983965
C	3.922409	-0.264222	1.574147
C	4.049675	0.242219	2.860310
C	2.899037	0.703916	3.535551
N	1.691003	0.648066	2.964026
C	2.952965	1.264412	4.910331
C	4.166148	1.567621	5.552322
C	4.179701	2.087064	6.844749
C	2.981122	2.314316	7.524571
C	1.769553	2.021453	6.895376
C	1.754196	1.505187	5.602150
C	-1.927464	-2.240092	0.956445
C	-1.529820	-2.920314	-0.371128
C	-2.251224	2.886662	1.308246
C	-2.028912	3.855185	0.126949
C	-2.757279	-3.201321	1.832291
C	-3.152248	3.514514	2.374113
H	-2.700337	4.432195	2.768274
H	-3.318828	2.829074	3.210806

H	-4.131200	3.781122	1.957869
H	-1.559791	3.346579	-0.721520
H	-1.386630	4.692995	0.423172
H	-2.974946	4.282936	-0.226322
H	-2.521371	-4.245572	1.598561
H	-3.832632	-3.057373	1.688651
H	-2.554643	-3.041994	2.896141
H	-1.050817	-2.211863	-1.054616
H	-2.408371	-3.328236	-0.884342
H	-0.841549	-3.754832	-0.188678
H	-4.552370	2.401924	-0.062804
H	-5.492622	0.226325	-0.790880
H	-4.300159	-1.867733	-0.252444
H	2.521089	-0.698236	-0.020783
H	4.796105	-0.624224	1.037669
H	5.024117	0.267709	3.334384
H	0.199511	-0.272473	0.078597
H	0.830769	2.195996	7.414308
H	2.992341	2.718577	8.533133
H	5.128482	2.319255	7.320933
H	5.114584	1.416939	5.045686
H	0.818062	1.278070	5.102646
H	-1.274311	2.691034	1.762137
H	-1.000968	-2.023889	1.496335

N22Th (2b)
E = -972.157915
H = -971.725677
G = -971.806877

C	-2.354006	1.454262	-0.089304
C	-2.019930	0.359668	0.747681
C	-2.894647	-0.751418	0.875545
C	-4.042233	-0.781252	0.081570
C	-4.363228	0.264129	-0.782886
C	-3.531346	1.374103	-0.844614
N	-0.863238	0.370568	1.547112
C	0.284983	0.468763	1.004662
C	1.542659	0.524616	1.778183
C	2.755323	0.551538	1.078357
C	3.941957	0.601747	1.808923
C	3.880568	0.625477	3.193674
C	2.615501	0.596652	3.817635
N	1.478077	0.547970	3.115269
C	2.486069	0.623375	5.272238
C	3.451399	0.652801	6.248781
C	2.930634	0.673368	7.574493
C	1.565670	0.659898	7.610058
S	0.850894	0.619985	5.995190
C	-2.646251	-1.913769	1.828728
C	-1.408399	-2.752371	1.475353
C	-1.543845	2.744577	-0.142300

C	-2.381413	3.945642	0.326398
C	-2.627543	-1.480192	3.302980
C	-0.955038	3.002345	-1.537238
H	-0.349318	3.915927	-1.537139
H	-1.744659	3.127520	-2.286736
H	-0.320873	2.172365	-1.867048
H	-3.224787	4.137334	-0.346072
H	-1.766061	4.852265	0.354318
H	-2.784525	3.776425	1.329757
H	-2.549567	-2.361901	3.950030
H	-3.548580	-0.948737	3.565526
H	-1.779981	-0.822650	3.511084
H	-1.414312	-3.047319	0.420159
H	-1.391381	-3.665811	2.081294
H	-0.483629	-2.205824	1.676402
H	-3.801584	2.205701	-1.490920
H	-5.265330	0.219259	-1.387097
H	-4.703808	-1.641874	0.154080
H	2.763642	0.532326	-0.007686
H	4.902681	0.623462	1.302007
H	4.789204	0.668833	3.784529
H	0.410068	0.493587	-0.088765
H	4.514263	0.657789	6.033556
H	3.549368	0.696735	8.464851
H	0.911280	0.669816	8.471251
H	-3.514563	-2.575260	1.703144
H	-0.707919	2.657435	0.557194

N2Fu (2c)
E = -1037.149713
H = -1036.714441
G = -1036.795398

C	-2.701416	1.586519	0.638715
C	-2.003425	0.386508	0.929508
C	-2.563678	-0.876853	0.634129
C	-3.814167	-0.908057	0.000800
C	-4.491908	0.257607	-0.329837
C	-3.934023	1.495194	-0.006091
N	-0.776904	0.510898	1.611924
C	0.304088	0.150480	1.044916
C	1.629281	0.228810	1.697539
C	2.755138	-0.156827	0.960125
C	4.006839	-0.082694	1.571422
C	4.088967	0.367138	2.879457
C	2.900310	0.734490	3.545124
N	1.700204	0.663709	2.962188
C	2.952706	1.213802	4.923351
C	3.987703	1.404114	5.807722
C	3.408177	1.895967	7.012354
C	2.065764	1.969277	6.774746
O	1.780407	1.560693	5.519360

C	-1.903874	-2.189614	1.034811
C	-1.552106	-3.055858	-0.183737
C	-2.108956	2.925304	1.055527
C	-2.586073	4.108140	0.208053
C	-2.777870	-2.971653	2.028299
C	-2.377403	3.181190	2.548925
H	-1.912392	4.121730	2.866973
H	-1.967137	2.374593	3.162370
H	-3.455023	3.252727	2.738332
H	-2.440540	3.927653	-0.862654
H	-2.023668	5.008185	0.479120
H	-3.646315	4.331821	0.373888
H	-2.259453	-3.877553	2.363095
H	-3.726493	-3.279849	1.574523
H	-3.009412	-2.365775	2.909898
H	-0.898198	-2.520847	-0.880803
H	-2.450357	-3.351629	-0.737611
H	-1.039620	-3.972478	0.130616
H	-4.473024	2.402575	-0.261065
H	-5.455199	0.207386	-0.830444
H	-4.263127	-1.870074	-0.234839
H	2.649879	-0.503749	-0.063943
H	4.904323	-0.372689	1.032206
H	5.048454	0.435146	3.381683
H	0.316151	-0.235078	0.013178
H	5.036580	1.217067	5.625866
H	3.917400	2.158992	7.928732
H	1.220852	2.278248	7.371713
H	-1.021654	2.855279	0.932408
H	-0.969349	-1.958840	1.554063

N23Th (2d)
E = -972.156319
H = -971.724115
G = -971.805783

C	3.597467	-3.122709	0.899329
C	3.594396	-2.285768	-0.185635
C	3.902258	-2.979309	-1.409458
C	4.130760	-4.308597	-1.241349
S	3.975715	-4.789384	0.461808
C	3.300656	-0.845563	-0.060604
C	3.246950	0.003453	-1.182864
C	2.956499	1.348815	-0.996632
C	2.726955	1.818273	0.293947
C	2.803495	0.906404	1.355758
N	3.081613	-0.389340	1.178849
C	2.565539	1.401365	2.728339
N	2.700363	0.672601	3.764467
C	2.421110	1.200529	5.038104

C	3.458871	1.164323	6.006148
C	3.195949	1.686771	7.273656
C	1.941642	2.190489	7.613984
C	0.919777	2.158448	6.674662
C	1.126432	1.667054	5.378891
C	4.844448	0.590042	5.738208
C	4.812218	-0.909931	5.405895
C	-0.067481	1.582440	4.434905
C	-0.634943	2.968037	4.092839
C	-1.163811	0.668505	5.005511
C	5.652278	1.377364	4.695043
H	4.296973	-1.090248	4.459162
H	4.298075	-1.473850	6.191573
H	5.834766	-1.297088	5.324654
H	5.247773	1.242056	3.688644
H	6.690820	1.026476	4.684744
H	5.660320	2.448797	4.923687
H	-1.464316	2.879855	3.381689
H	0.127514	3.617348	3.649268
H	-1.016249	3.475250	4.986210
H	-0.767732	-0.326115	5.233073
H	-1.979296	0.553527	4.282148
H	-1.593304	1.077124	5.927073
H	3.993732	1.686730	8.013293
H	1.760909	2.586562	8.609600
H	-0.068190	2.518937	6.950803
H	2.496224	2.863199	0.481199
H	2.908226	2.023035	-1.847312
H	3.423719	-0.382510	-2.180885
H	2.283359	2.463075	2.798915
H	3.956909	-2.507992	-2.383913
H	4.381619	-5.057938	-1.978940
H	3.398927	-2.864383	1.929410
H	5.383825	0.692825	6.689774
H	0.263419	1.123173	3.499267

N2H (2e)
E = -808.395654
H = -808.014969
G = -808.085126

C	1.071405	-0.803092	3.745743
C	1.239975	-0.493647	2.388876
N	2.450074	-0.372584	1.818964
C	3.517564	-0.559571	2.590189
C	3.453653	-0.871045	3.953422
C	2.198656	-0.994683	4.541141
C	0.034075	-0.296797	1.557721
N	0.078413	-0.030704	0.313166
C	-1.111906	0.167647	-0.410007

C	-1.338912	-0.699541	-1.508017
C	-2.501683	-0.533743	-2.259900
C	-3.407569	0.485678	-1.970310
C	-3.141589	1.364204	-0.926564
C	-1.998321	1.234994	-0.127456
C	-0.348073	-1.812475	-1.804589
C	-0.746826	-3.110754	-1.083471
C	-1.725167	2.281962	0.944587
C	-2.789034	2.265614	2.052483
C	-1.594198	3.686206	0.333291
C	-0.147274	-2.063717	-3.302848
H	0.670019	-2.777079	-3.456354
H	0.106558	-1.139660	-3.832431
H	-1.039663	-2.490500	-3.775465
H	-0.837238	-2.957154	-0.003185
H	0.002641	-3.893066	-1.251526
H	-1.711762	-3.480728	-1.450444
H	-2.534606	4.019494	-0.119581
H	-0.822849	3.706692	-0.442902
H	-1.320931	4.415133	1.104968
H	-3.779907	2.517268	1.657571
H	-2.546359	2.997380	2.831758
H	-2.865591	1.279090	2.522315
H	-2.701663	-1.205732	-3.089689
H	-4.308209	0.602890	-2.567115
H	-3.834727	2.177943	-0.727228
H	4.483639	-0.455367	2.098014
H	4.364640	-1.010072	4.527822
H	2.097177	-1.235497	5.595778
H	-0.922629	-0.412875	2.090594
H	0.072026	-0.891422	4.163946
H	0.613000	-1.487338	-1.386958
H	-0.761793	2.053021	1.409260

Yb(II)N2Ph
E = -2893.188179
H = -2892.443078
G = -2892.563197

Yb	1.216775	2.262759	1.530745
C	1.337536	5.077047	1.432113
C	1.207564	4.672163	2.795008
C	-0.087997	4.124200	2.950997
C	-0.749808	4.100859	1.702385
C	0.120638	4.699725	0.744528
C	2.345266	5.779601	0.726472
C	2.159368	6.076956	-0.609077
C	0.981025	5.675484	-1.292930
C	-0.024747	4.994044	-0.635834
C	3.237045	0.419678	0.686685

C	3.065400	-0.984659	0.689309
C	2.583883	-1.616256	-0.443568
C	2.255159	-0.875756	-1.607863
C	2.386335	0.500140	-1.636179
C	2.875149	1.179830	-0.493473
C	3.204595	2.546023	-0.247019
C	3.810201	2.610954	1.027656
C	3.796330	1.334936	1.630080
C	-3.576756	1.342062	-1.174790
C	-4.631997	1.706370	-0.347011
C	-4.444577	1.732791	1.030368
C	-3.213118	1.407075	1.608568
C	-2.150337	1.046491	0.744109
C	-2.321755	1.007800	-0.654466
N	-0.868039	0.751529	1.325293
C	-0.756285	-0.397457	1.892163
C	0.336183	-0.752562	2.799794
C	0.469127	-2.092167	3.181499
C	1.428464	-2.426364	4.127213
C	2.180647	-1.402631	4.693041
C	1.982939	-0.076259	4.277020
N	1.096365	0.244618	3.311633
C	2.708756	1.015342	4.967354
C	4.043751	0.855364	5.371039
C	4.697629	1.866306	6.070279
C	4.023190	3.046104	6.391860
C	2.694406	3.210805	6.001983
C	2.043390	2.205322	5.289155
C	-3.074901	1.435413	3.126570
C	-3.662992	2.703329	3.764139
C	-1.225254	0.518979	-1.583178
C	-1.066659	1.383305	-2.839492
C	-3.716965	0.188336	3.761454
C	-1.474493	-0.950532	-1.966512
H	-4.793971	0.162595	3.559846
H	-3.577332	0.192950	4.848527
H	-3.290426	-0.739902	3.368171
H	-3.246474	3.612958	3.323382
H	-3.442052	2.715296	4.837270
H	-4.752628	2.746024	3.660833
H	-2.423202	-1.056461	-2.506006
H	-1.520997	-1.594379	-1.081923
H	-0.670076	-1.320467	-2.609880
H	-0.896400	2.434016	-2.586289
H	-1.946013	1.328357	-3.490852
H	-0.210509	1.034176	-3.425339
H	-5.272552	2.016583	1.673747
H	-5.598065	1.964165	-0.772402
H	-3.731239	1.305849	-2.249279
H	-0.174063	-2.845268	2.736556

H	1.566246	-3.455997	4.443802
H	2.886494	-1.610890	5.489827
H	-1.541028	-1.153894	1.779315
H	2.160386	4.122430	6.255008
H	4.532156	3.832349	6.942371
H	5.736827	1.735846	6.358936
H	4.584431	-0.050575	5.109454
H	1.004925	2.326677	4.998767
H	3.249751	6.099811	1.239369
H	2.924393	6.628576	-1.149879
H	0.866769	5.924728	-2.344976
H	-0.940006	4.721866	-1.157288
H	-1.761281	3.767242	1.512374
H	-0.518930	3.786619	3.888411
H	1.930138	4.853707	3.581166
H	1.912579	-1.405069	-2.493574
H	2.480001	-2.698564	-0.455222
H	3.352202	-1.569078	1.561433
H	2.155974	1.058832	-2.540510
H	3.084873	3.372902	-0.936502
H	4.200827	3.513790	1.483944
H	4.233399	1.081500	2.586826
H	-2.006573	1.424312	3.368870
H	-0.272561	0.550696	-1.042220

Yb(III)N2Ph
E = -2893.173584
H = -2892.428757
G = -2892.546762

Yb	1.168836	2.020217	1.519516
C	1.528684	4.795065	1.554435
C	1.207100	4.300575	2.858267
C	-0.122975	3.827843	2.818040
C	-0.611495	3.899030	1.491151
C	0.402519	4.518342	0.693474
C	2.641320	5.510564	1.053312
C	2.640953	5.915251	-0.267304
C	1.556870	5.602732	-1.128973
C	0.452835	4.912105	-0.668045
C	2.910180	0.140658	0.340452
C	2.572085	-1.182386	-0.031797
C	2.193648	-1.435258	-1.335438
C	2.110248	-0.389130	-2.291505
C	2.374390	0.921101	-1.945684
C	2.785219	1.212501	-0.620882
C	3.268728	2.409638	-0.003990
C	3.744909	2.059017	1.286397
C	3.476184	0.693032	1.530811
C	0.397313	-0.659586	2.911598

C	0.627083	-1.949920	3.462332
C	1.502390	-2.102268	4.508222
C	2.138776	-0.955786	5.035238
C	1.888454	0.284186	4.458469
N	1.075661	0.452767	3.388113
C	-0.569469	-0.472362	1.896246
N	-0.768392	0.712101	1.291261
C	-2.080277	0.917346	0.761256
C	-3.148528	1.166707	1.666575
C	-4.426200	1.415119	1.155971
C	-4.672509	1.428511	-0.212355
C	-3.626105	1.172283	-1.089074
C	-2.329482	0.907521	-0.630771
C	2.516695	1.485857	5.076521
C	3.910087	1.619187	5.142177
C	4.488413	2.704079	5.802024
C	3.680860	3.657908	6.422800
C	2.291809	3.524588	6.376187
C	1.714293	2.449596	5.701770
C	-2.957224	1.177755	3.177301
C	-3.548310	2.434206	3.836152
C	-1.264036	0.543362	-1.648931
C	-1.130246	1.586920	-2.764926
C	-3.548343	-0.085009	3.824309
C	-1.550448	-0.846292	-2.240912
H	-4.630419	-0.141990	3.657045
H	-3.375424	-0.081169	4.906875
H	-3.099943	-0.994439	3.412766
H	-3.171675	3.351333	3.372668
H	-3.291168	2.458524	4.901598
H	-4.641655	2.454424	3.768476
H	-2.511531	-0.857463	-2.768237
H	-1.590572	-1.610650	-1.458263
H	-0.769871	-1.130347	-2.954444
H	-0.908877	2.579304	-2.360572
H	-2.045486	1.666143	-3.362188
H	-0.318011	1.310928	-3.444903
H	-5.243867	1.607648	1.846086
H	-5.671275	1.629874	-0.590548
H	-3.820966	1.162753	-2.158425
H	0.093594	-2.798829	3.044024
H	1.686412	-3.081420	4.941465
H	2.789138	-1.019280	5.900734
H	-1.212159	-1.320298	1.651339
H	1.656904	4.256797	6.867906
H	4.131243	4.497317	6.945573
H	5.570399	2.799780	5.836287
H	4.542038	0.869957	4.672514
H	0.634098	2.338368	5.674979
H	3.475264	5.754573	1.707164

H	3.481389	6.483130	-0.657933
H	1.590372	5.933679	-2.163668
H	-0.389330	4.715573	-1.326472
H	-1.593980	3.595404	1.153242
H	-0.668796	3.417544	3.658949
H	1.829622	4.383890	3.739502
H	1.832563	-0.629732	-3.314370
H	1.964327	-2.452693	-1.641083
H	2.656027	-1.991829	0.688977
H	2.312706	1.715376	-2.685360
H	3.347547	3.380778	-0.474922
H	4.209859	2.743315	1.987957
H	3.737939	0.137019	2.421195
H	-1.881763	1.178161	3.375049
H	-0.301616	0.482074	-1.129676

Yb(II)N22Th
E = -2825.974563
H = -2825.263488
G = -2825.381245

Yb	-0.030458	2.151672	3.377803
C	-0.784623	3.675077	5.448966
C	0.250393	2.911559	6.026360
C	-0.257256	1.595300	6.233823
C	-1.607700	1.553066	5.707701
C	-1.909143	2.853390	5.198846
C	-2.366920	0.365202	5.850518
C	-1.817895	-0.726621	6.497014
C	-0.502149	-0.676565	7.026967
C	0.268974	0.462942	6.899661
C	1.018234	2.948455	0.955987
C	1.590882	3.955042	1.789868
C	0.510270	4.755627	2.318504
C	-0.709784	4.242554	1.777595
C	-0.376487	3.180668	0.913831
C	0.806051	5.869177	3.141170
C	2.123070	6.186981	3.415664
C	3.184920	5.413340	2.879716
C	2.930915	4.313378	2.081296
N	-1.481987	0.350899	2.071322
C	-1.252162	-0.872750	2.392506
C	-0.140972	-1.314931	3.237104
C	-0.057783	-2.679315	3.535184
C	1.052562	-3.151481	4.225171
C	2.037868	-2.246731	4.589257
C	1.873164	-0.885200	4.283234
N	0.800302	-0.419931	3.607951
C	2.894412	0.074808	4.675841
S	2.975153	1.631457	3.814593

C	4.263132	2.178379	4.895646
C	4.610622	1.211131	5.791192
C	3.833022	0.019939	5.672954
C	-2.450692	0.511504	1.017413
C	-3.752286	0.964825	1.308454
C	-4.662028	1.097145	0.254020
C	-4.301352	0.803839	-1.055966
C	-3.007363	0.373744	-1.327498
C	-2.058146	0.214545	-0.311238
C	-4.202143	1.267312	2.725696
C	-4.844991	2.653148	2.848876
C	-0.657739	-0.259267	-0.678503
C	-0.053075	0.517750	-1.854913
C	-5.151317	0.175350	3.241565
C	-0.642740	-1.766155	-0.989243
H	-5.450857	0.376502	4.276567
H	-4.678657	-0.812248	3.210692
H	-6.063117	0.126763	2.635481
H	-4.165723	3.437585	2.501593
H	-5.101101	2.858927	3.893912
H	-5.769075	2.726579	2.265336
H	-1.244632	-1.982916	-1.879355
H	-1.051857	-2.362660	-0.167547
H	0.379707	-2.110182	-1.183289
H	-0.056413	1.596477	-1.674663
H	-0.591424	0.328183	-2.789755
H	0.985142	0.204919	-2.011174
H	-5.673431	1.433042	0.465990
H	-5.023366	0.912772	-1.860561
H	-2.723386	0.157005	-2.353193
H	-0.847787	-3.350313	3.212802
H	1.155609	-4.207018	4.458569
H	2.939808	-2.576309	5.092959
H	-1.867275	-1.678371	1.977260
H	3.940110	-0.827604	6.341227
H	5.390959	1.348645	6.531676
H	4.664546	3.171418	4.751899
H	-0.718354	4.731800	5.219747
H	-2.864907	3.188844	4.816032
H	1.213054	3.285601	6.355256
H	1.264947	0.507596	7.333928
H	-3.393709	0.322565	5.496502
H	-2.412051	-1.627703	6.630877
H	-0.109187	-1.540483	7.557889
H	0.000904	6.489730	3.529473
H	-1.694898	4.673827	1.910797
H	-1.083660	2.633944	0.303160
H	1.569745	2.233535	0.356432
H	3.753165	3.752659	1.640348
H	4.212001	5.712199	3.078307

H	2.352812	7.052570	4.031878
H	-3.311730	1.258007	3.359707
H	-0.007589	-0.088210	0.184195

Yb(III)N22Th
E = -2825.956970
H = -2825.246735
G = -2825.365053

Yb	-0.158734	1.898472	3.320536
C	-1.437811	3.243849	5.122331
C	-0.119263	3.121003	5.632296
C	0.011923	1.799841	6.166353
C	-1.215593	1.095909	5.898305
C	-2.089124	1.997915	5.211243
C	-1.395645	-0.221063	6.375452
C	-0.391392	-0.803920	7.124402
C	0.814132	-0.109881	7.396750
C	1.030129	1.167415	6.918284
C	1.128659	2.975703	1.272399
C	1.426703	3.996638	2.233633
C	0.189152	4.649411	2.574569
C	-0.853128	4.019084	1.820465
C	-0.250453	3.066073	0.977355
C	0.196831	5.759793	3.450729
C	1.398163	6.207845	3.964596
C	2.618908	5.568414	3.628608
C	2.641986	4.479179	2.779040
N	-1.622172	0.521210	2.047277
C	-1.563056	-0.764310	2.435846
C	-0.504661	-1.304384	3.197626
C	-0.516948	-2.687022	3.516710
C	0.577723	-3.266351	4.110980
C	1.693546	-2.458580	4.397490
C	1.633988	-1.094433	4.128076
N	0.558237	-0.490344	3.550706
C	2.774694	-0.256288	4.470877
S	2.868698	1.360514	3.739500
C	4.298198	1.751914	4.713195
C	4.679758	0.680787	5.464521
C	3.817343	-0.450330	5.338258
C	-2.441017	0.718450	0.890132
C	-3.659250	1.435923	0.968063
C	-4.430618	1.593853	-0.187206
C	-4.026652	1.062299	-1.407755
C	-2.822943	0.372371	-1.482164
C	-2.008050	0.193776	-0.357561
C	-4.162414	1.970051	2.295625
C	-4.946645	3.282558	2.187535
C	-0.677774	-0.531757	-0.533024

C	0.186167	0.097854	-1.639085
C	-4.997681	0.903381	3.023055
C	-0.879416	-2.029366	-0.809616
H	-5.346535	1.271468	3.995631
H	-4.417346	-0.009158	3.190717
H	-5.880283	0.636093	2.430002
H	-4.400020	4.036589	1.611474
H	-5.136334	3.689093	3.187082
H	-5.923183	3.140896	1.710992
H	-1.430617	-2.186401	-1.744105
H	-1.441846	-2.515434	-0.006587
H	0.087348	-2.537723	-0.900788
H	0.341642	1.168310	-1.472902
H	-0.268491	-0.021564	-2.628676
H	1.168720	-0.386652	-1.671198
H	-5.368158	2.139344	-0.130872
H	-4.642109	1.192903	-2.293869
H	-2.501396	-0.032984	-2.438170
H	-1.392499	-3.273678	3.253999
H	0.594028	-4.328605	4.336796
H	2.595756	-2.885106	4.819976
H	-2.323159	-1.463096	2.082158
H	3.942175	-1.357566	5.917678
H	5.551517	0.700987	6.109837
H	4.753303	2.725646	4.605802
H	-1.867138	4.149820	4.712582
H	-3.114043	1.786732	4.939606
H	0.606142	3.921578	5.710852
H	1.955517	1.692783	7.139920
H	-2.322138	-0.754235	6.178373
H	-0.525093	-1.808516	7.516706
H	1.580375	-0.595667	7.995413
H	-0.730519	6.273453	3.693840
H	-1.893616	4.318352	1.797193
H	-0.771979	2.478234	0.234817
H	1.851441	2.354527	0.757277
H	3.588379	4.031148	2.483511
H	3.550299	5.962600	4.027438
H	1.415246	7.072899	4.622349
H	-3.276676	2.165730	2.908107
H	-0.120128	-0.438325	0.403494

Yb(II)N2Fu
E = -2890.976343
H = -2890.262361
G = -2890.378190

C	3.278416	3.895338	2.344304
C	1.937115	3.643800	1.969395
C	0.901537	4.581918	2.352323

C	1.240931	5.709824	3.137170
C	2.560733	5.925276	3.489735
C	3.580286	5.026732	3.081787
C	1.333373	2.644946	1.146059
C	-0.020035	3.014081	0.964729
C	-0.316640	4.157645	1.735648
Yb	-0.024813	2.114514	3.480861
C	-0.278326	1.839119	6.289960
C	-1.607928	1.626871	5.750448
C	-2.028909	2.853477	5.149970
C	-0.997119	3.798000	5.350557
C	0.094474	3.185167	6.001640
C	0.361131	0.794780	7.000060
C	-0.285315	-0.416009	7.166524
C	-1.580977	-0.629679	6.628650
C	-2.236026	0.369518	5.932194
N	-1.584262	0.373580	2.031991
C	-1.301995	-0.855269	2.278166
C	-0.182991	-1.292131	3.108294
C	-0.016504	-2.666076	3.295692
C	1.094794	-3.119606	4.001368
C	1.996548	-2.185890	4.481382
C	1.758756	-0.817190	4.259364
N	0.684526	-0.367282	3.580188
C	2.697347	0.160972	4.766448
C	3.861345	0.072001	5.487155
C	4.298732	1.406093	5.721296
C	3.381192	2.221781	5.129215
O	2.408767	1.476495	4.539417
C	-2.540182	0.579597	0.980136
C	-3.841687	1.018191	1.299146
C	-4.755291	1.207327	0.257212
C	-4.400945	0.979977	-1.066963
C	-3.115308	0.545318	-1.364768
C	-2.159343	0.332372	-0.365069
C	-4.291876	1.185779	2.741350
C	-5.105043	-0.040616	3.195589
C	-0.776283	-0.169080	-0.771613
C	-0.812652	-1.660672	-1.152507
C	-0.154545	0.639334	-1.919990
C	-5.081544	2.478386	2.980796
H	-5.409080	0.059875	4.243801
H	-4.523890	-0.963823	3.097317
H	-6.012655	-0.152937	2.591451
H	-4.524491	3.356000	2.637491
H	-5.292481	2.601347	4.048417
H	-6.047171	2.469067	2.463919
H	-1.486301	-1.827767	-2.000762
H	-1.164522	-2.289447	-0.328676
H	0.185459	-2.010115	-1.440728

H	-0.168648	1.713561	-1.714593
H	-0.670660	0.468011	-2.870617
H	0.887645	0.334648	-2.060881
H	-5.767024	1.525457	0.490297
H	-5.123768	1.135785	-1.863319
H	-2.843942	0.368897	-2.401513
H	-0.746264	-3.358000	2.886667
H	1.254964	-4.180613	4.167077
H	2.879056	-2.498124	5.028345
H	-1.858888	-1.662404	1.789588
H	4.345139	-0.833889	5.822948
H	5.179129	1.723013	6.261780
H	3.289336	3.290318	5.013882
H	-1.032995	4.835988	5.039666
H	-3.003308	3.066845	4.730834
H	1.007311	3.680388	6.309460
H	1.344231	0.958204	7.437178
H	-3.243325	0.200150	5.557232
H	-2.072310	-1.586871	6.786871
H	0.194847	-1.211890	7.730980
H	0.473611	6.424715	3.426521
H	-1.263204	4.685070	1.760311
H	-0.735541	2.494565	0.342610
H	1.850227	1.835477	0.642914
H	4.069513	3.219252	2.025551
H	4.614183	5.240961	3.343814
H	2.827660	6.806180	4.068368
H	-3.388228	1.226051	3.360939
H	-0.114493	-0.053557	0.094645

Yb(III)N2Fu
E = -2890.959998
H = -2890.245011
G = -2890.357335

C	2.706213	4.511477	2.940196
C	1.568801	3.898804	2.358769
C	0.268392	4.493189	2.550255
C	0.137332	5.649129	3.355572
C	1.262360	6.206601	3.930820
C	2.547052	5.645073	3.714717
C	1.414664	2.803603	1.446499
C	0.065970	2.796903	1.023164
C	-0.663938	3.763473	1.744559
Yb	-0.045652	1.785197	3.412128
C	0.090056	1.677053	6.244888
C	-1.150924	1.011921	5.940280
C	-1.991769	1.953644	5.266420
C	-1.302325	3.179886	5.204069

C	0.004998	3.011137	5.730472
C	1.079449	0.993863	6.992272
C	0.832471	-0.298231	7.411976
C	-0.383814	-0.955996	7.095889
C	-1.366586	-0.319233	6.364160
N	-1.643276	0.513293	2.106720
C	-1.600707	-0.792612	2.422167
C	-0.519908	-1.367328	3.121743
C	-0.443908	-2.765443	3.347167
C	0.705899	-3.315752	3.863732
C	1.789037	-2.470282	4.180011
C	1.641337	-1.101217	3.992205
N	0.522608	-0.533682	3.481439
C	2.706405	-0.185121	4.359303
C	3.962054	-0.330845	4.881697
C	4.477703	0.982563	5.089175
C	3.511255	1.847643	4.681893
O	2.429964	1.152260	4.215880
C	-2.463978	0.783273	0.966179
C	-3.621011	1.594567	1.069072
C	-4.395075	1.827243	-0.071485
C	-4.057545	1.278742	-1.303768
C	-2.914268	0.496372	-1.404151
C	-2.095769	0.241333	-0.297593
C	-4.075714	2.136250	2.410970
C	-4.952283	1.102243	3.136577
C	-0.827648	-0.580200	-0.515229
C	-1.152892	-2.054521	-0.805255
C	0.053871	-0.017140	-1.642705
C	-4.792945	3.487924	2.333049
H	-5.266285	1.472083	4.120394
H	-4.416553	0.158851	3.279670
H	-5.856878	0.889683	2.554887
H	-4.224384	4.218453	1.747773
H	-4.934898	3.895456	3.340129
H	-5.788346	3.402412	1.882396
H	-1.744586	-2.148393	-1.723560
H	-1.728602	-2.512254	0.004487
H	-0.232912	-2.635060	-0.938415
H	0.301860	1.036882	-1.485425
H	-0.432171	-0.099233	-2.621095
H	0.992931	-0.579646	-1.699290
H	-5.287896	2.440470	0.008911
H	-4.676167	1.464531	-2.177598
H	-2.640818	0.081196	-2.371078
H	-1.293254	-3.385663	3.075590
H	0.785863	-4.387548	4.019474
H	2.711161	-2.869428	4.586076
H	-2.372603	-1.465362	2.041788
H	4.456039	-1.264796	5.107013

H	5.442166	1.251638	5.496220
H	3.423374	2.921365	4.650968
H	-1.696751	4.105482	4.803563
H	-3.016946	1.774511	4.976837
H	0.745264	3.795495	5.840702
H	2.011548	1.489247	7.252425
H	-2.302186	-0.822362	6.133911
H	-0.541881	-1.973899	7.441925
H	1.581078	-0.823302	7.999743
H	-0.835823	6.116350	3.488980
H	-1.713685	3.993380	1.612303
H	-0.358446	2.126061	0.290063
H	2.213014	2.191594	1.042989
H	3.700102	4.124258	2.727313
H	3.418958	6.135638	4.140343
H	1.170853	7.106517	4.533306
H	-3.170866	2.278130	3.008599
H	-0.241067	-0.539684	0.406148

Yb(II)N23Th
E = -2825.971355
H = -2825.260399
G = -2825.378914

C	-3.112163	2.736524	2.745890
C	-3.066588	3.979959	3.462277
C	-4.209502	4.205852	4.187782
S	-5.374443	2.892619	4.028928
C	-4.265418	2.042247	2.937841
C	-1.934934	4.920042	3.446505
N	-0.687204	4.433428	3.279644
C	0.335700	5.320261	3.278436
C	0.158884	6.694935	3.462583
C	-1.128140	7.192075	3.623103
C	-2.185047	6.295748	3.594308
Yb	0.133664	1.940367	3.498293
C	0.936589	1.082331	5.915405
C	0.656099	2.446135	6.240653
C	-0.778472	2.631660	6.143364
C	-1.350854	1.387012	5.745253
C	-0.302462	0.444859	5.666454
C	1.464846	3.525749	6.674926
C	0.879594	4.731920	7.010807
C	-0.527453	4.904096	6.938304
C	-1.345568	3.874634	6.515791
C	1.688691	4.857980	2.964761
N	2.030878	3.626453	2.825436
C	3.308193	3.405127	2.216454
C	4.334748	2.766072	2.946148
C	5.554159	2.523042	2.308167

C	5.766643	2.889146	0.984148
C	4.746679	3.513578	0.277319
C	3.504424	3.785765	0.862024
C	4.185311	2.437899	4.421097
C	4.926164	3.486938	5.267915
C	2.435972	4.455807	0.000676
C	2.237022	3.754447	-1.353921
C	1.368450	-0.023358	2.071328
C	1.128473	1.031033	1.167293
C	-0.257561	1.134242	0.898864
C	-0.898888	0.047642	1.573143
C	0.116797	-0.670600	2.313185
C	-0.235908	-1.842962	3.023552
C	-1.541057	-2.295626	2.989211
C	-2.533903	-1.602466	2.250227
C	-2.225112	-0.449558	1.553507
C	4.663162	1.024498	4.777029
C	2.757245	5.941952	-0.234190
H	4.529959	4.493675	5.099645
H	4.835689	3.260134	6.336111
H	5.993590	3.501439	5.018984
H	4.158164	0.265599	4.171986
H	4.453603	0.812972	5.830989
H	5.743011	0.907038	4.633998
H	3.702380	6.053015	-0.777593
H	2.854194	6.499697	0.702926
H	1.970126	6.416437	-0.831249
H	2.055487	2.682528	-1.238579
H	3.106086	3.880360	-2.008515
H	1.375332	4.188917	-1.872402
H	6.356762	2.046985	2.864139
H	6.721624	2.689384	0.505976
H	4.914000	3.792919	-0.759131
H	1.021897	7.353408	3.457675
H	-1.304442	8.256462	3.746648
H	-3.209761	6.644590	3.658148
H	2.415219	5.655595	2.776012
H	-0.430455	-0.604518	5.428699
H	1.901232	0.592715	5.977232
H	-2.407304	1.173561	5.633215
H	-2.425188	4.001135	6.498897
H	2.537082	3.393807	6.789919
H	1.499427	5.550901	7.368298
H	-0.964428	5.851563	7.244941
H	0.524464	-2.398216	3.569013
H	2.339382	-0.364417	2.410317
H	1.898618	1.662064	0.744917
H	-0.718630	1.804456	0.181181
H	-2.980741	0.044287	0.944570
H	-3.544989	-2.001419	2.216660

H	-1.811698	-3.205214	3.519448
H	-4.439625	5.023963	4.855757
H	-4.561094	1.086096	2.532490
H	-2.329615	2.393087	2.075378
H	3.120110	2.499585	4.670773
H	1.478588	4.396696	0.528515

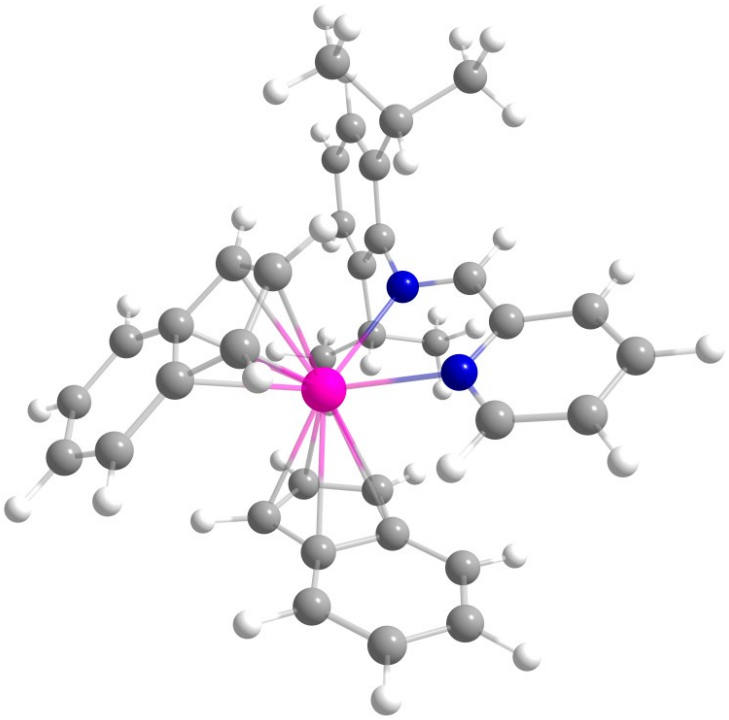
Yb(III)N23Th
E = -2825.957987
H = -2825.247424
G = -2825.364350

C	-3.270941	3.270349	1.791141
C	-3.103790	4.015356	3.008418
C	-4.166040	3.866164	3.858413
S	-5.407509	2.789642	3.199609
C	-4.436470	2.570742	1.731767
C	-1.957950	4.914953	3.273639
N	-0.702710	4.406099	3.173492
C	0.358617	5.278505	3.360150
C	0.141119	6.639738	3.699286
C	-1.137137	7.125008	3.808009
C	-2.216824	6.245875	3.577780
Yb	0.135251	2.141945	3.404118
C	0.642634	1.102686	5.722226
C	0.583342	2.474885	6.140792
C	-0.781465	2.919347	5.985689
C	-1.537190	1.822462	5.465411
C	-0.675068	0.707631	5.389065
C	1.542074	3.351421	6.707405
C	1.150470	4.609931	7.114929
C	-0.192544	5.044177	6.966720
C	-1.146875	4.221354	6.407537
C	1.671430	4.798002	3.159602
N	1.934669	3.514631	2.860120
C	3.187716	3.275336	2.216537
C	4.219331	2.566987	2.878745
C	5.411322	2.305211	2.194239
C	5.607380	2.733704	0.887197
C	4.598445	3.445471	0.248288
C	3.384100	3.729308	0.882572
C	4.111842	2.169351	4.341056
C	4.941177	3.130933	5.209670
C	2.332675	4.527030	0.116898
C	2.101680	4.008590	-1.312322
C	1.430210	0.298733	1.979777
C	0.794954	1.192147	1.095498
C	-0.608498	1.026378	1.181196
C	-0.858112	-0.076593	2.061735
C	0.420764	-0.542098	2.544846

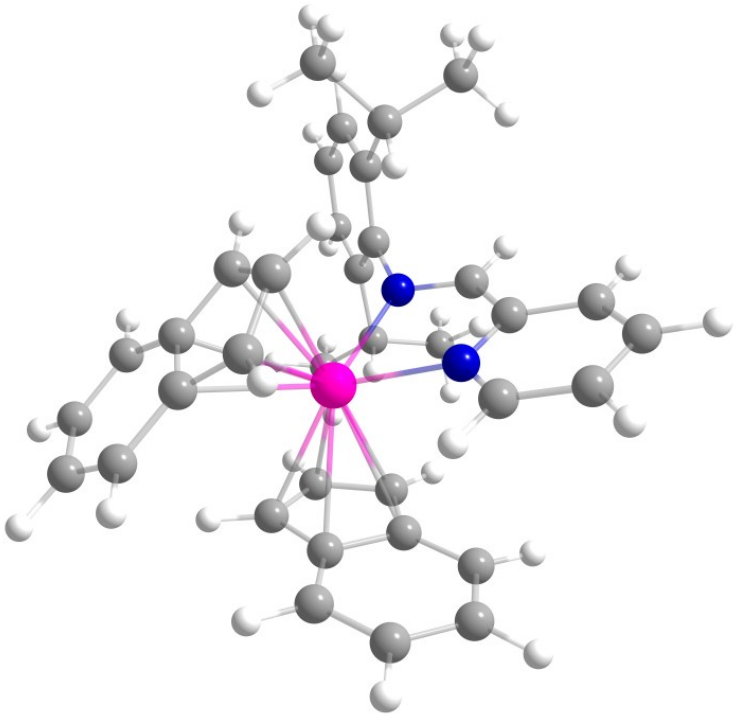
C	0.486628	-1.705026	3.350427
C	-0.678945	-2.377428	3.657709
C	-1.940841	-1.905223	3.205940
C	-2.040413	-0.769287	2.428615
C	4.523745	0.716233	4.611314
C	2.698319	6.020578	0.062444
H	4.590839	4.162675	5.106626
H	4.880831	2.853357	6.268519
H	5.997563	3.104411	4.918022
H	3.961876	0.012259	3.989541
H	4.342044	0.460061	5.661328
H	5.589758	0.550919	4.420541
H	3.642349	6.167654	-0.475095
H	2.816432	6.447411	1.062253
H	1.920635	6.589724	-0.459785
H	1.892801	2.934557	-1.338167
H	2.968550	4.190205	-1.956953
H	1.249965	4.529118	-1.764559
H	6.208279	1.768579	2.702365
H	6.540422	2.521209	0.372135
H	4.756488	3.785962	-0.771633
H	1.003761	7.280896	3.855641
H	-1.318469	8.167626	4.052886
H	-3.243193	6.594117	3.602040
H	2.486898	5.520618	3.206335
H	-0.972183	-0.288013	5.085052
H	1.501115	0.445946	5.797127
H	-2.602929	1.812082	5.272769
H	-2.175821	4.557820	6.316333
H	2.565258	3.020654	6.859103
H	1.876623	5.276860	7.572714
H	-0.470464	6.037167	7.309500
H	1.447709	-2.078768	3.694948
H	2.499981	0.198503	2.111705
H	1.304534	1.922408	0.482361
H	-1.343646	1.522868	0.563408
H	-3.008284	-0.426980	2.072083
H	-2.838702	-2.457083	3.471140
H	-0.636507	-3.284552	4.254822
H	-4.312486	4.292344	4.840926
H	-4.827773	1.957550	0.931847
H	-2.556792	3.312659	0.978230
H	3.063006	2.282454	4.635024
H	1.384728	4.434273	0.657080

Yb(II)N2H
E = -2662.222123
H = -2661.562402
G = -2661.671961

Yb	-0.742908	0.332447	-1.054797
C	0.529950	-0.162794	-3.468280
C	-0.743313	-0.779335	-3.489456
C	1.351342	-0.908863	-2.569966
C	0.527983	-1.950349	-1.988493
C	-0.773791	-1.848103	-2.565917
C	2.730251	-0.852116	-2.255555
C	3.267229	-1.777299	-1.378963
C	2.452456	-2.769711	-0.771231
C	1.102957	-2.856293	-1.061309
C	-3.204555	-0.269784	-0.021505
C	-4.215653	-0.732904	-0.903880
C	-4.384118	-2.091064	-1.089757
C	-3.552692	-3.030190	-0.422770
C	-2.534806	-2.613724	0.411994
C	-2.329495	-1.227703	0.626110
C	-1.423544	-0.495649	1.452037
C	-1.774934	0.870567	1.359657
C	-2.835375	1.029954	0.435962
N	1.269170	1.450987	-0.145418
C	1.442892	2.770293	-0.398173
C	2.601538	3.456535	-0.018124
C	3.610401	2.767474	0.648493
C	3.427012	1.411602	0.913973
C	2.248006	0.798028	0.492559
C	0.350604	3.494353	-1.039441
N	-0.726986	2.923381	-1.461985
C	-1.783940	3.788270	-1.880335
C	-2.232871	3.710825	-3.219975
C	-3.295308	4.524066	-3.618274
C	-3.916553	5.389639	-2.724358
C	-3.466190	5.456212	-1.412266
C	-2.398928	4.673710	-0.955750
C	-1.508478	2.844175	-4.234084
C	-2.439487	2.183411	-5.256174
C	-1.968293	4.833091	0.499092
C	-3.140369	4.721288	1.488077
C	-0.411506	3.655726	-4.946237
C	-1.237577	6.170229	0.718462
H	2.082137	-0.260986	0.671552
H	-0.849697	4.485599	-5.512774
H	0.143051	3.021616	-5.646728
H	0.303122	4.080095	-4.233179
H	-3.253306	1.637769	-4.767680
H	-1.875768	1.474446	-5.871566
H	-2.885997	2.913751	-5.939949
H	-1.901231	7.014515	0.500734
H	-0.359988	6.276232	0.072451
H	-0.907754	6.262347	1.759311
H	-3.707972	3.798419	1.348072



H	-3.835238	5.562948	1.394448
H	-2.760102	4.728702	2.515395
H	-3.640687	4.483894	-4.646920
H	-4.745986	6.011148	-3.050564
H	-3.955134	6.134919	-0.718650
H	2.697706	4.515406	-0.240384
H	4.518376	3.277747	0.956045
H	4.180760	0.827955	1.432051
H	0.473431	4.579377	-1.113402
H	3.366255	-0.100920	-2.719775
H	4.331588	-1.754443	-1.156404
H	2.903949	-3.483041	-0.085994
H	0.492006	-3.637387	-0.615384
H	-1.617008	-2.497246	-2.366180
H	-1.574402	-0.485825	-4.122578
H	0.864435	0.647924	-4.104762
H	-3.724217	-4.092813	-0.575797
H	-5.172029	-2.451813	-1.746172
H	-4.876973	-0.023159	-1.397188
H	-1.907121	-3.342027	0.921000
H	-0.681294	-0.923316	2.116628
H	-1.297556	1.673618	1.911537
H	-3.324530	1.956652	0.164618
H	-1.004888	2.044963	-3.678829
H	-1.273421	4.023144	0.743822



Yb(III)N2H
E = -2662.208047
H = -2661.549040
G = -2661.657823

Yb	-0.694072	0.553180	-1.079015
C	0.437749	-1.774806	-1.916251
C	-0.857200	-1.610218	-2.502097
C	-0.770727	-0.547536	-3.430647
C	0.527742	0.013543	-3.391018
C	1.306505	-0.770307	-2.485519
C	0.965158	-2.713699	-0.990712
C	2.311280	-2.678202	-0.690036
C	3.168879	-1.706257	-1.273426
C	2.682613	-0.756086	-2.145792
C	-3.104716	-0.215388	-0.097591
C	-4.130463	-0.686880	-0.957293
C	-4.301117	-2.048185	-1.115436
C	-3.462697	-2.975035	-0.441965
C	-2.424972	-2.546697	0.362711
C	-2.213105	-1.158511	0.538356
C	-1.293130	-0.409007	1.340942
C	-1.684075	0.946871	1.282264
C	-2.749727	1.091316	0.362706

N	1.218871	1.545648	-0.161139
C	1.405461	2.850039	-0.582338
C	2.599579	3.544517	-0.245365
C	3.545969	2.942698	0.549583
C	3.321862	1.623080	1.011090
C	2.164270	0.980808	0.613651
C	0.358939	3.473007	-1.295348
N	-0.807685	2.858724	-1.577772
C	-1.867172	3.725640	-1.980622
C	-2.340961	3.690165	-3.314679
C	-3.411121	4.513207	-3.676387
C	-4.004862	5.373125	-2.760377
C	-3.520552	5.421222	-1.458707
C	-2.458217	4.613182	-1.039038
C	-1.638261	2.856046	-4.371822
C	-2.591001	2.194627	-5.373133
C	-1.972199	4.735023	0.404043
C	-3.109668	4.648533	1.435490
C	-0.578674	3.700605	-5.101896
C	-1.191404	6.043299	0.613654
H	1.974045	-0.046771	0.913799
H	-1.049224	4.523300	-5.652666
H	-0.019720	3.088081	-5.820099
H	0.136647	4.135785	-4.396639
H	-3.385581	1.632154	-4.870650
H	-2.040037	1.503419	-6.020702
H	-3.069569	2.929499	-6.029804
H	-1.832015	6.914054	0.431424
H	-0.333489	6.118171	-0.061106
H	-0.819809	6.109867	1.642563
H	-3.708780	3.741857	1.316785
H	-3.787620	5.506201	1.365763
H	-2.697746	4.646173	2.450841
H	-3.775062	4.497059	-4.700063
H	-4.836487	6.005626	-3.060451
H	-3.982609	6.102763	-0.749810
H	2.734610	4.559811	-0.607840
H	4.452802	3.474749	0.823444
H	4.039121	1.110653	1.642436
H	0.491358	4.519092	-1.574237
H	3.345923	-0.013903	-2.582402
H	4.226197	-1.714037	-1.021953
H	2.729962	-3.412620	-0.006685
H	0.321278	-3.476951	-0.563044
H	-1.726442	-2.228339	-2.319617
H	-1.585595	-0.213054	-4.063141
H	0.894929	0.831491	-3.998889
H	-3.645862	-4.039475	-0.563558
H	-5.102241	-2.420517	-1.748371
H	-4.799803	0.015680	-1.448349

H	-1.797411	-3.265566	0.883244
H	-0.528314	-0.826025	1.985282
H	-1.201914	1.758881	1.813554
H	-3.243420	2.015384	0.090180
H	-1.284603	3.905255	0.593277
H	-1.096056	2.067939	-3.842926

Yb(Cp*2) with the same Ipy ligands

Yb(Cp*2)
E = -1939.650074
H = -1939.179828
G = -1939.270840

C	-0.379794	1.733867	0.251920
C	0.395914	3.020714	0.163833
C	0.706758	3.885270	1.255653
C	0.316773	3.664956	2.692428
C	1.336752	5.051534	0.728863
C	1.416324	4.907785	-0.688104
C	0.834059	3.653501	-1.037608
Yb	3.040088	3.056521	0.312263
C	5.260791	1.840858	1.087454
C	5.153350	1.585260	-0.312036
C	5.337015	2.820550	-1.001328
C	5.558658	3.839483	-0.028015
C	5.511597	3.234364	1.262716
C	5.246913	0.801386	2.175701
C	5.007383	0.231175	-0.952196
C	5.428669	2.991725	-2.493138
C	5.925612	5.269359	-0.316312
C	5.806487	3.922112	2.568191
C	0.602538	3.150903	-2.436800
C	1.896208	5.957116	-1.652982
C	1.718178	6.278063	1.512085
H	1.384549	3.480112	-3.130413
H	0.566446	2.056425	-2.484368
H	-0.351859	3.513417	-2.844354
H	-0.136784	1.046160	-0.566297
H	-0.197151	1.198363	1.191352
H	-1.463615	1.909748	0.200587
H	0.274027	2.600783	2.952577
H	1.013803	4.142576	3.390885
H	-0.677621	4.079392	2.910836
H	1.986836	6.041876	2.547945
H	2.570509	6.804224	1.067907
H	0.890975	7.000493	1.558714
H	2.683277	6.584448	-1.220656

H	2.298745	5.519970	-2.573518
H	1.082057	6.631994	-1.953313
H	4.785554	2.287559	-3.033490
H	5.142856	4.000549	-2.810348
H	6.452457	2.824519	-2.856801
H	4.418805	-0.460827	-0.337877
H	4.523032	0.287452	-1.933842
H	5.983449	-0.248432	-1.112489
H	4.902843	1.207288	3.134157
H	4.599973	-0.049771	1.931462
H	6.249808	0.388255	2.354131
H	5.495976	4.973120	2.562129
H	5.303526	3.439782	3.414303
H	6.881642	3.913651	2.796911
H	5.473286	5.632318	-1.245588
H	5.610088	5.947096	0.484723
H	7.012665	5.393252	-0.423561

Yb(Cp*2)(THF)2
E = -2404.428175
H = -2403.707089
G = -2403.824408

Yb	0.662849	1.223448	0.485264
C	1.125990	3.927406	0.334502
C	1.478489	3.574968	1.669194
C	2.096138	3.352377	-0.535524
C	2.657935	2.780567	1.623758
C	3.040335	2.642150	0.258983
C	-1.317661	-0.505921	-0.382496
C	-1.572230	0.724552	-1.053751
C	-0.518883	0.947465	-1.982651
C	0.400547	-0.133715	-1.875808
C	-0.102801	-1.039231	-0.896404
C	0.434127	-2.419103	-0.643851
O	-0.947668	1.341548	2.535748
C	-2.007224	2.313853	2.429655
C	-2.448534	2.592586	3.858310
C	-2.268763	1.217216	4.507613
C	-1.012946	0.686084	3.816211
O	1.985407	-0.633450	1.717833
C	1.503109	-1.590036	2.679533
C	2.491984	-2.749462	2.654161
C	3.800331	-2.037759	2.301836
C	3.327234	-0.980046	1.312236
H	-2.822137	1.889771	1.831602
H	-1.595414	3.180914	1.908122
H	-0.102424	0.936364	4.375481

H	-1.045530	-0.395662	3.655549
H	-3.128555	0.575575	4.285490
H	-2.153227	1.262758	5.594105
H	4.233499	-1.565043	3.190590
H	4.552387	-2.703075	1.868913
H	2.530329	-3.282360	3.608522
H	2.222259	-3.466273	1.871433
H	1.478960	-1.109831	3.666868
H	0.486097	-1.877571	2.397966
H	3.925018	-0.068508	1.319480
H	3.291191	-1.372168	0.287859
H	-3.476573	2.961808	3.910988
H	-1.791811	3.332889	4.326697
C	0.065021	4.914899	-0.069763
C	0.891271	4.142944	2.929410
C	3.429401	2.348229	2.839435
C	4.325846	2.075039	-0.281125
C	-2.264516	-1.202400	0.554132
C	-2.843158	1.527873	-1.000547
C	-0.552179	1.992628	-3.060045
C	1.580016	-0.386228	-2.773258
C	2.297107	3.671301	-1.989006
H	-0.062532	4.649216	2.746370
H	0.720788	3.381742	3.701217
H	1.559193	4.895313	3.375116
H	-0.217084	4.796626	-1.120900
H	-0.859728	4.822474	0.514467
H	0.407034	5.953242	0.052008
H	4.347336	1.814065	2.573082
H	3.737852	3.213226	3.443850
H	2.856625	1.689583	3.507089
H	4.180994	1.251843	-0.994315
H	4.900153	2.845924	-0.813391
H	4.976744	1.702640	0.517174
H	1.389399	4.057184	-2.459279
H	3.073105	4.441865	-2.116183
H	2.622464	2.801635	-2.571360
H	1.528609	-2.459593	-0.687651
H	0.131170	-2.814546	0.331874
H	0.067957	-3.134561	-1.395236
H	-2.740755	-0.510953	1.259525
H	-3.075974	-1.710888	0.012786
H	-1.761164	-1.972091	1.150327
H	-3.499221	1.197196	-0.188476
H	-2.671928	2.604604	-0.869436
H	-3.420795	1.418350	-1.930210
H	-0.861753	2.975675	-2.686622
H	0.418643	2.117508	-3.546021

H	-1.269504	1.716260	-3.847784
H	2.018174	0.546026	-3.144107
H	2.380741	-0.936201	-2.263643
H	1.304954	-0.982455	-3.656215

Yb(II)N2Ph
E = -2979.016984
H = -2978.077823
G = -2978.219329

Yb	1.202549	2.482741	1.303132
C	1.568369	5.168918	1.823671
C	1.787222	4.537485	3.081369
C	2.654291	4.828468	0.971871
C	-0.525318	1.128122	-0.315093
C	0.773346	0.783573	-0.788021
C	-0.750725	2.501893	-0.619645
C	1.346958	1.939657	-1.388551
C	0.397365	2.995766	-1.298755
C	2.626364	1.954783	-2.177318
C	2.992713	3.781289	2.996096
C	3.521665	3.957390	1.686236
C	4.896125	3.573826	1.218274
N	-0.067902	1.735613	3.862733
C	0.880726	1.080989	4.572829
C	0.968182	1.131817	5.969544
C	0.037401	1.879766	6.678769
C	-0.981745	2.494839	5.964573
C	-1.016437	2.390324	4.563038
C	1.775454	0.139721	3.892668
N	1.970525	0.051929	2.624521
C	2.566083	-1.194574	2.223949
C	1.786853	-2.377686	2.323273
C	2.362892	-3.584618	1.911806
C	3.659993	-3.644482	1.419317
C	4.408706	-2.477137	1.333127
C	3.885010	-1.241196	1.725287
C	0.352806	-2.407703	2.845439
C	0.282847	-3.004970	4.261574
C	4.779405	-0.015504	1.701532
C	5.690562	-0.009629	2.941499
C	-2.215005	2.919077	3.864523
C	-2.751051	4.175111	4.187449
C	-3.958289	4.593702	3.632205
C	-4.661444	3.751649	2.769250
C	-4.139310	2.498343	2.449611
C	-2.918046	2.089054	2.982683
C	-0.598061	-3.177843	1.915556
C	5.624251	0.085761	0.425435
H	0.643078	-4.039968	4.263757
H	-0.750265	-3.007708	4.627542
H	0.893652	-2.445432	4.976971
H	-0.544053	-2.812290	0.886691
H	-1.631426	-3.064063	2.261328

H	-0.377147	-4.250588	1.904118
H	6.360312	-0.877322	2.926450
H	5.112525	-0.055270	3.870248
H	6.310209	0.893655	2.969010
H	5.005075	0.027479	-0.474664
H	6.372875	-0.711854	0.369975
H	6.165997	1.035655	0.405223
H	1.778300	-4.497905	1.977517
H	4.085663	-4.594261	1.107241
H	5.427782	-2.527254	0.961594
H	1.750833	0.577073	6.478797
H	0.079775	1.946357	7.761905
H	-1.782107	3.018825	6.476172
H	2.228009	-0.599482	4.564879
H	-4.684682	1.835325	1.783429
H	-5.610120	4.071410	2.347209
H	-4.352050	5.576117	3.877724
H	-2.216402	4.832272	4.868109
H	-2.512581	1.112191	2.740487
C	1.318957	-0.609598	-0.908243
C	-1.544425	0.150429	0.200367
C	-2.036003	3.268859	-0.490933
C	3.026827	5.492634	-0.320579
C	0.494598	6.184263	1.546202
C	1.063196	4.900665	4.343290
H	-0.015239	-1.378239	2.895799
H	4.134906	0.871494	1.752068
C	3.714353	3.142541	4.148109
C	0.420775	4.288544	-2.061405
H	0.902809	-1.283729	-0.155655
H	1.081112	-1.040083	-1.893024
H	2.408110	-0.652288	-0.802535
H	3.039321	2.963460	-2.276939
H	3.402884	1.332485	-1.718290
H	2.478064	1.568651	-3.196736
H	1.417059	4.530041	-2.438039
H	-0.243721	4.225654	-2.936110
H	0.075046	5.143287	-1.469325
H	-2.711733	2.826873	0.243935
H	-1.868693	4.308418	-0.185129
H	-2.576903	3.306377	-1.448654
H	-2.499525	0.644775	0.399914
H	-1.746656	-0.637019	-0.538979
H	-1.237172	-0.356580	1.123362
H	3.365230	4.782640	-1.082812
H	2.200023	6.064727	-0.746411
H	3.855042	6.198678	-0.158788
H	0.336851	6.328452	0.473162
H	-0.472338	5.898132	1.977391
H	0.748576	7.168786	1.966721
H	-0.011357	5.034379	4.182052
H	1.189826	4.153481	5.131414
H	1.438008	5.853618	4.746980
H	4.156875	2.174185	3.889634
H	4.536864	3.778117	4.508165

H	3.050560	2.976635	5.001714
H	5.369128	2.855391	1.893432
H	4.898680	3.138527	0.211963
H	5.557113	4.452768	1.179507

Yb(III)N2Ph
E = -2979.010734
H = -2978.072649
G = -2978.208769

Yb	1.255689	2.340664	1.501598
C	1.640743	4.992578	1.921064
C	1.880782	4.374507	3.179278
C	2.708670	4.629502	1.049309
C	-0.503601	1.132506	-0.090280
C	0.790792	0.853518	-0.636807
C	-0.770502	2.510593	-0.286300
C	1.311166	2.060076	-1.181650
C	0.334701	3.077564	-0.990171
C	2.547512	2.147628	-2.030981
C	3.086440	3.615517	3.081104
C	3.588334	3.763720	1.760736
C	4.976442	3.422651	1.300643
N	-0.095125	1.813783	3.577217
C	0.850052	1.166722	4.364144
C	0.780219	1.193841	5.786236
C	-0.279951	1.795837	6.412825
C	-1.293245	2.361055	5.611739
C	-1.164669	2.339528	4.225159
C	1.854655	0.373675	3.762670
N	2.035945	0.223005	2.438135
C	2.598058	-1.053971	2.106423
C	1.830842	-2.230377	2.348373
C	2.370005	-3.477736	2.014351
C	3.635740	-3.604087	1.456273
C	4.390493	-2.457628	1.249130
C	3.902692	-1.187177	1.572607
C	0.436278	-2.211527	2.966110
C	0.463059	-2.696467	4.425203
C	4.847802	-0.009288	1.443753
C	5.881682	-0.048257	2.582897
C	-2.351369	2.847377	3.471418
C	-2.616882	4.215185	3.341247
C	-3.829440	4.656907	2.808558
C	-4.801530	3.736084	2.418315
C	-4.550922	2.369453	2.554231
C	-3.334367	1.929770	3.075149
C	-0.574682	-3.048951	2.165747
C	5.566879	0.043736	0.089818
H	0.810363	-3.734720	4.482585
H	-0.540147	-2.652615	4.865087
H	1.130037	-2.089080	5.043743
H	-0.576708	-2.782797	1.104861
H	-1.586139	-2.891542	2.557394
H	-0.364281	-4.121523	2.239124

H	6.493468	-0.955656	2.514574
H	5.398827	-0.053192	3.565264
H	6.559235	0.812407	2.536557
H	4.861045	0.049565	-0.746341
H	6.233715	-0.814180	-0.050091
H	6.186030	0.944193	0.020343
H	1.781292	-4.372604	2.197848
H	4.034044	-4.582763	1.201904
H	5.395210	-2.550700	0.845405
H	1.563864	0.699088	6.353308
H	-0.356452	1.812069	7.496443
H	-2.186250	2.789762	6.052909
H	2.459602	-0.222414	4.449940
H	-5.305964	1.643924	2.262592
H	-5.750944	4.080769	2.017725
H	-4.019040	5.722778	2.712341
H	-1.878985	4.936608	3.678062
H	-3.148609	0.867293	3.203558
C	1.358841	-0.511849	-0.879106
C	-1.457389	0.108157	0.448056
C	-2.075815	3.227566	-0.112490
C	3.098208	5.342558	-0.211950
C	0.591559	6.033473	1.630211
C	1.175046	4.726905	4.456054
H	0.084230	-1.175946	2.967099
H	4.251617	0.903353	1.555817
C	3.825329	2.993213	4.230498
C	0.231149	4.383697	-1.720464
H	0.967094	-1.255016	-0.181804
H	1.108542	-0.847946	-1.896289
H	2.448678	-0.538214	-0.793295
H	2.804588	3.181709	-2.271757
H	3.423386	1.699505	-1.549850
H	2.405696	1.617942	-2.983324
H	1.126676	4.603413	-2.304477
H	-0.606696	4.335318	-2.430690
H	0.028509	5.238376	-1.066339
H	-2.754065	2.700715	0.558836
H	-1.944815	4.238316	0.286884
H	-2.584690	3.332855	-1.081576
H	-2.426445	0.557879	0.673568
H	-1.630579	-0.686104	-0.289826
H	-1.094539	-0.373131	1.360223
H	3.823911	4.767852	-0.794363
H	2.253579	5.568350	-0.860021
H	3.577940	6.300041	0.039107
H	0.767198	6.497845	0.655963
H	-0.433655	5.644307	1.621228
H	0.621981	6.839302	2.375118
H	0.193670	5.167505	4.265233
H	1.030575	3.873768	5.123530
H	1.758222	5.474162	5.013157
H	4.284390	2.036716	3.963294
H	4.631344	3.653982	4.580472
H	3.162399	2.811670	5.080304

H	5.453666	2.691415	1.955302
H	5.004217	3.028432	0.279843
H	5.609452	4.321380	1.311176

Yb(II)N2Fu
E = -2976.804772
H = -2975.896796
G = -2976.035832

Yb	-3.392554	-1.742313	1.135409
C	-6.039133	-1.542268	0.360832
C	-6.020972	-2.636847	1.270280
C	-5.278199	-3.696584	0.673547
C	-4.848952	-3.258331	-0.611765
C	-5.328616	-1.933986	-0.807658
C	-2.397827	0.805535	0.656873
C	-2.046533	0.026759	-0.483348
C	-1.101069	-0.955634	-0.076291
C	-0.863671	-0.779256	1.315983
C	-1.660831	0.307649	1.769431
C	-3.207978	2.073418	0.605853
C	-2.365305	0.395055	-1.903244
C	-1.547255	0.927401	3.133299
C	0.188102	-1.464741	2.136280
C	-0.346499	-1.874994	-0.995350
C	-6.843265	-2.736984	2.522031
C	-5.157768	-5.093327	1.211957
C	-4.243615	-4.111630	-1.689438
C	-5.352641	-1.215834	-2.124601
C	-6.863928	-0.292527	0.497920
O	-4.372941	-0.673665	3.246975
C	-4.519110	-1.319594	4.441351
C	-5.149404	-0.482909	5.327893
C	-5.421757	0.727476	4.630492
C	-4.932235	0.562038	3.371260
C	-4.044750	-2.689459	4.544741
C	-4.449385	-3.424821	5.673562
C	-4.008572	-4.726417	5.829279
C	-3.141341	-5.236464	4.870155
C	-2.768695	-4.446058	3.774898
N	-3.245237	-3.191161	3.576038
C	-1.710201	-5.040634	2.940270
N	-1.157084	-4.546572	1.898881
C	0.035326	-5.188543	1.459811
C	0.074296	-5.749528	0.159524
C	1.265598	-6.315863	-0.295996
C	2.408717	-6.332332	0.497700
C	2.359354	-5.784294	1.771563
C	1.190508	-5.208781	2.287622

C	-1.187760	-5.834334	-0.676043
C	-0.938743	-5.748787	-2.184578
C	1.250014	-4.638946	3.701129
C	2.429731	-3.672607	3.898744
C	-1.951002	-7.128113	-0.337452
C	1.321967	-5.759478	4.752821
H	-2.885189	-7.191255	-0.906813
H	-2.198603	-7.186454	0.727330
H	-1.343220	-8.005632	-0.586891
H	-0.344922	-4.867785	-2.447123
H	-1.892215	-5.687255	-2.718355
H	-0.418942	-6.635849	-2.563942
H	2.234078	-6.353341	4.624548
H	0.474889	-6.449788	4.682466
H	1.336227	-5.338868	5.765069
H	2.446581	-2.895427	3.130964
H	3.392554	-4.194679	3.873072
H	2.352326	-3.183598	4.876308
H	1.300572	-6.755297	-1.287944
H	3.329858	-6.771845	0.124835
H	3.252993	-5.800356	2.389615
H	-2.733772	-6.237842	4.966191
H	-4.318789	-5.324216	6.680893
H	-5.115821	-2.973478	6.399594
H	-1.341074	-5.988155	3.354805
H	-5.389357	-0.698922	6.358816
H	-5.909814	1.611535	5.014888
H	-4.893566	1.184718	2.492443
H	-3.944825	-5.088447	-1.301085
H	-4.965004	-4.297772	-2.498324
H	-3.360091	-3.658821	-2.156059
H	-5.421156	-0.130138	-2.006707
H	-4.467145	-1.424339	-2.731957
H	-6.226726	-1.525256	-2.718018
H	-7.065151	-0.043852	1.545511
H	-6.380397	0.579527	0.041072
H	-7.843203	-0.398797	0.007962
H	-6.429458	-3.454486	3.238525
H	-6.941535	-1.775869	3.039503
H	-7.865657	-3.075898	2.298230
H	-5.303094	-5.125764	2.296381
H	-5.912063	-5.762758	0.772503
H	-4.179351	-5.540150	1.003996
H	-4.227587	1.928500	0.221675
H	-3.286985	2.542886	1.592423
H	-2.738552	2.818479	-0.051584
H	-1.444674	0.174835	3.924504
H	-0.662986	1.577985	3.202980
H	-2.412768	1.546994	3.389405
H	0.516790	-2.396915	1.671605

H	1.077326	-0.826778	2.253088
H	-0.159825	-1.707145	3.147385
H	-2.343553	-0.468685	-2.575511
H	-3.349257	0.862085	-2.002913
H	-1.629420	1.115474	-2.292096
H	-0.014432	-2.786747	-0.488550
H	-0.952358	-2.181838	-1.855506
H	0.554147	-1.390931	-1.400956
H	0.338363	-4.062375	3.882767
H	-1.819132	-4.985013	-0.387415

Yb(III)N2Fu
E = -2976.791169
H = -2975.882565
G = -2976.017355

Yb	-3.219854	-2.030107	1.329401
C	-5.888808	-1.737593	0.692620
C	-5.749024	-2.964824	1.397569
C	-5.005303	-3.864933	0.576827
C	-4.676036	-3.186148	-0.628904
C	-5.230733	-1.870629	-0.555552
C	-2.476345	0.505340	0.551702
C	-1.992157	-0.376365	-0.471092
C	-0.996141	-1.203482	0.095961
C	-0.856158	-0.844209	1.468407
C	-1.755310	0.220692	1.744381
C	-3.337949	1.710215	0.296676
C	-2.218407	-0.224769	-1.946623
C	-1.729635	1.006853	3.023643
C	0.196062	-1.334248	2.408635
C	-0.074378	-2.080742	-0.694549
C	-6.469884	-3.335579	2.658585
C	-4.830699	-5.326457	0.863662
C	-4.134471	-3.809397	-1.882916
C	-5.436842	-0.948642	-1.720958
C	-6.841975	-0.629927	1.034526
O	-4.382614	-0.563945	3.207992
C	-4.439573	-1.099668	4.470627
C	-4.997161	-0.182926	5.320698
C	-5.308531	0.970436	4.540837
C	-4.919033	0.692902	3.269698
C	-3.969975	-2.467260	4.615251
C	-4.284527	-3.149256	5.780186
C	-3.908195	-4.506604	5.898755
C	-3.201820	-5.072470	4.867613
C	-2.838822	-4.310658	3.723794
N	-3.278336	-2.998667	3.565405
C	-1.923443	-4.894109	2.820761
N	-1.379843	-4.319117	1.755142
C	-0.171157	-4.960687	1.347415

C	-0.041590	-5.524738	0.049889
C	1.167979	-6.104442	-0.341169
C	2.259743	-6.165235	0.516168
C	2.128399	-5.649750	1.797208
C	0.942502	-5.050340	2.242696
C	-1.228301	-5.634982	-0.888701
C	-0.875593	-5.456097	-2.369854
C	0.937724	-4.544751	3.685733
C	2.171635	-3.688897	4.024716
C	-1.912448	-6.999527	-0.684606
C	0.857881	-5.706902	4.692390
H	-2.815744	-7.089337	-1.301435
H	-2.191403	-7.156705	0.361497
H	-1.230366	-7.808512	-0.971086
H	-0.283553	-4.553417	-2.546757
H	-1.787770	-5.389246	-2.972324
H	-0.304395	-6.307575	-2.756665
H	1.726614	-6.367811	4.592059
H	-0.037305	-6.317807	4.548415
H	0.844187	-5.324130	5.719725
H	2.349134	-2.904935	3.284238
H	3.081478	-4.295835	4.089147
H	2.036723	-3.208829	5.000890
H	1.251727	-6.534810	-1.335029
H	3.192735	-6.619905	0.193901
H	2.972102	-5.713399	2.479046
H	-2.871442	-6.106348	4.920076
H	-4.170225	-5.080393	6.782352
H	-4.851465	-2.655828	6.560901
H	-1.598520	-5.899948	3.100185
H	-5.161316	-0.313839	6.380230
H	-5.759101	1.891545	4.882497
H	-4.951214	1.237623	2.342697
H	-3.864807	-4.854247	-1.721761
H	-4.893175	-3.794972	-2.676985
H	-3.250695	-3.296478	-2.279215
H	-5.295609	0.107190	-1.467526
H	-4.769070	-1.178989	-2.552994
H	-6.466730	-1.045313	-2.093890
H	-7.011631	-0.536030	2.110194
H	-6.506684	0.343530	0.661381
H	-7.822010	-0.819701	0.573113
H	-5.937476	-4.099454	3.231639
H	-6.623096	-2.475503	3.316933
H	-7.465599	-3.739907	2.425791
H	-4.680068	-5.519059	1.929373
H	-5.722189	-5.890130	0.553718
H	-3.975948	-5.749810	0.336125
H	-4.347719	1.462774	-0.051728
H	-3.437155	2.329875	1.192539

H	-2.888821	2.349501	-0.474303
H	-1.873679	0.381324	3.912253
H	-0.756720	1.502493	3.142621
H	-2.492547	1.787357	3.050839
H	0.590549	-2.295973	2.082304
H	1.036078	-0.626282	2.459603
H	-0.183048	-1.457501	3.429016
H	-2.430508	-1.177094	-2.444933
H	-3.042875	0.455170	-2.170028
H	-1.318339	0.186870	-2.425016
H	0.415772	-2.836199	-0.078762
H	-0.595873	-2.602510	-1.502367
H	0.715717	-1.476323	-1.163839
H	0.054619	-3.916575	3.827829
H	-1.934662	-4.849393	-0.599758

Yb(II)N2H
E = -2748.061475
H = -2747.207779
G = -2747.337899

Yb	-0.849246	-0.017473	-1.007514
C	0.227505	-2.374616	-1.762666
C	1.164741	-1.369014	-2.138618
C	0.596392	-0.614924	-3.204889
C	-0.695283	-1.149163	-3.481075
C	-0.915182	-2.247578	-2.605868
C	-2.900892	-1.154195	0.405594
C	-2.065814	-0.519266	1.369103
C	-2.190808	0.888017	1.198302
C	-3.099076	1.121303	0.126043
C	-3.528174	-0.138846	-0.374705
N	-0.888888	2.270417	-1.978869
C	-1.890629	2.471874	-2.848361
C	-2.219030	3.711021	-3.387124
C	-1.481836	4.827809	-2.988404
C	-0.433998	4.636403	-2.098577
C	-0.145087	3.346633	-1.624945
C	1.063469	3.175210	-0.819749
N	1.506164	2.056449	-0.364982
C	2.842162	2.073976	0.135044
C	3.090563	1.649376	1.463258
C	4.406112	1.620829	1.930107
C	5.473126	1.992700	1.120473
C	5.222127	2.408821	-0.179141
C	3.924809	2.464376	-0.703614

C	1.957861	1.352189	2.428274
C	1.676301	2.595906	3.289994
C	3.781262	2.923445	-2.152268
C	4.081492	4.424649	-2.300548
C	2.228131	0.134934	3.320854
C	4.673513	2.118007	-3.111085
C	-3.698654	2.456360	-0.202918
H	-2.464403	1.590622	-3.126372
H	2.562291	2.862906	3.877588
H	0.851444	2.412197	3.986627
H	1.412083	3.460692	2.672923
H	2.454648	-0.758072	2.729714
H	1.353316	-0.079922	3.943037
H	3.066472	0.306864	4.004463
H	5.118629	4.644687	-2.024029
H	3.439792	5.039513	-1.660733
H	3.936726	4.745282	-3.338539
H	4.518896	1.041317	-2.998892
H	5.736653	2.321680	-2.944559
H	4.448432	2.386860	-4.148995
H	4.599579	1.313820	2.953495
H	6.490159	1.962381	1.501699
H	6.056694	2.698948	-0.811501
H	0.182405	5.470902	-1.776570
H	-1.713535	5.817656	-3.369880
H	-3.038449	3.792444	-4.093835
H	1.638167	4.098055	-0.674947
C	-3.269128	-2.609560	0.407654
C	-1.354057	-1.221266	2.492405
C	-1.674278	1.952371	2.123081
C	-1.572353	-0.776367	-4.644860
C	1.294720	0.429937	-4.025564
C	2.565733	-1.255971	-1.609609
H	1.059823	1.147812	1.833487
H	2.747860	2.759019	-2.470897
C	-4.615306	-0.350698	-1.392922
C	-2.029647	-3.241995	-2.757970
C	0.496164	-3.478968	-0.777454
H	-3.725813	-2.917038	-0.535699
H	-2.410615	-3.266645	0.584086
H	-4.000492	-2.824126	1.200690
H	-4.638156	0.445005	-2.147061
H	-4.503077	-1.298711	-1.928987
H	-5.611423	-0.365967	-0.926748
H	-2.976236	3.274839	-0.105875
H	-4.105743	2.495532	-1.218848
H	-4.534272	2.688105	0.474415
H	-1.059843	1.521532	2.917998
H	-1.067417	2.716841	1.619640
H	-2.501628	2.483522	2.614384

H	-1.225712	-2.287330	2.279737
H	-0.357811	-0.812460	2.688297
H	-1.916183	-1.149937	3.434983
H	-0.418171	-4.018572	-0.513071
H	1.200089	-4.219750	-1.182985
H	0.934311	-3.112977	0.159546
H	-3.010783	-2.767681	-2.873681
H	-1.873373	-3.862385	-3.652462
H	-2.094065	-3.922718	-1.905868
H	-1.411480	0.258671	-4.967458
H	-1.370086	-1.408619	-5.522380
H	-2.639067	-0.892052	-4.416966
H	2.121419	0.884169	-3.474659
H	1.720581	0.000946	-4.944478
H	0.624068	1.239984	-4.335545
H	2.949275	-0.232711	-1.654437
H	2.639966	-1.576668	-0.564211
H	3.263515	-1.887788	-2.179222

Yb(III)N2H
E = -2748.056063
H = -2747.201588
G = -2747.327419

Yb	-0.609649	0.244730	-0.958756
C	0.337836	-2.216929	-1.385532
C	1.304285	-1.296141	-1.883102
C	0.749624	-0.652680	-3.028297
C	-0.555945	-1.180812	-3.238933
C	-0.800551	-2.164721	-2.245800
C	-2.686795	-0.865741	0.387398
C	-1.902280	-0.187306	1.359514
C	-2.013160	1.213344	1.113067
C	-2.869597	1.395748	-0.009549
C	-3.271464	0.114418	-0.473331
N	-0.956409	2.168736	-2.282498
C	-1.846738	2.380986	-3.268098
C	-2.161406	3.626558	-3.780659
C	-1.540166	4.759858	-3.201951
C	-0.632253	4.576805	-2.187197
C	-0.303840	3.262652	-1.745329
C	0.742874	3.049820	-0.821185
N	1.200917	1.839554	-0.438889
C	2.549290	1.878763	0.034945
C	2.898357	1.325998	1.296819
C	4.223375	1.385599	1.738842
C	5.222539	1.983096	0.983776
C	4.887233	2.521060	-0.250428
C	3.582381	2.476262	-0.754899
C	1.880673	0.734258	2.255696

C	1.705203	1.651055	3.478076
C	3.384620	3.049750	-2.157301
C	3.508745	4.583174	-2.177658
C	2.261931	-0.682020	2.710982
C	4.380215	2.459648	-3.172777
C	-3.441054	2.718032	-0.424390
H	-2.339759	1.493193	-3.654783
H	2.642350	1.728066	4.040745
H	0.943651	1.258746	4.162883
H	1.413140	2.662574	3.180933
H	2.410592	-1.353919	1.860800
H	1.482974	-1.110297	3.349694
H	3.190701	-0.679545	3.291223
H	4.513160	4.895270	-1.869174
H	2.795691	5.066260	-1.503609
H	3.333436	4.969273	-3.188498
H	4.408716	1.366665	-3.136346
H	5.400069	2.818752	-2.997031
H	4.101728	2.760122	-4.189240
H	4.474514	0.973524	2.712750
H	6.244445	2.028821	1.350410
H	5.666165	2.980751	-0.852996
H	-0.130007	5.422940	-1.726366
H	-1.776601	5.759645	-3.555338
H	-2.881769	3.719208	-4.585934
H	1.260110	3.941674	-0.464464
C	-3.141843	-2.288508	0.535699
C	-1.358378	-0.841290	2.595872
C	-1.550271	2.330945	2.000920
C	-1.408302	-0.956646	-4.454596
C	1.457322	0.273302	-3.966361
C	2.731261	-1.212994	-1.421417
H	0.918973	0.686344	1.731740
H	2.378938	2.789531	-2.496994
C	-4.314503	-0.150128	-1.521372
C	-1.895801	-3.185962	-2.346407
C	0.593554	-3.221743	-0.296804
H	-3.678113	-2.645016	-0.345048
H	-2.319877	-2.983373	0.733222
H	-3.834386	-2.365489	1.386193
H	-4.383110	0.668470	-2.244506
H	-4.119122	-1.067859	-2.084407
H	-5.310751	-0.258280	-1.070052
H	-2.682510	3.502802	-0.498833
H	-3.950671	2.664219	-1.389516
H	-4.181595	3.055838	0.314272
H	-0.906532	1.972127	2.805519
H	-0.998865	3.103919	1.454123
H	-2.411702	2.823444	2.473025
H	-0.920130	-1.822985	2.388449

H	-0.595805	-0.233809	3.086985
H	-2.160826	-0.999409	3.330965
H	-0.308362	-3.785362	-0.044492
H	1.353121	-3.952014	-0.607587
H	0.958503	-2.764584	0.629637
H	-2.886626	-2.744475	-2.490916
H	-1.712014	-3.833414	-3.215478
H	-1.944365	-3.833938	-1.470140
H	-1.181794	-0.006146	-4.945895
H	-1.236381	-1.746402	-5.200322
H	-2.479990	-0.972459	-4.225335
H	2.372241	0.667812	-3.524034
H	1.742233	-0.248944	-4.890429
H	0.839417	1.129930	-4.256550
H	3.202526	-0.269552	-1.701379
H	2.831573	-1.305820	-0.336418
H	3.325315	-2.023572	-1.867236