Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information for:

Synthesis, structures, and coordination chemistry of a neutral pyrrolyl functionalized amidinate ligand

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Table S1 Crystallographic data for complexes **HL**, **1**, **2**, **3**, **4**

	HL	**1**	**2**	**3**	**4**
Formula	$C_{31}H_{35}N_3$	$C_{39}H_{50}N_3NaO_2$	$C_{78}H_{100}K_2N_6O_4$	$C_{43}H_{58}Cl_2N_3O_3Y$	$C_{43}H_{58}Cl_2N_3O_3Er$
FW	449.62	615.81	1263.83	824.73	903.08
Space group	P-1	P 1 2_1/n 1	P1 2_1/c 1	P-1	P-1
T (K)	298.15 K	298.15 K	298.15 K	298.15 K	298.15 K
Crystal system	Triclinic	Monoclinic	Monoclinic	triclinic	triclinic
a (Å)	9.2544(10)	12.6032(13)	32.8979(17)	11.362(2)	11.3647(11)
b (Å)	9.5728(11)	15.0919(15)	11.7923(7)	13.161(3)	13.1600(12)
c (Å)	15.8225(17)	20.395(2)	19.9051(12)	17.005(3)	17.0082(16)
α (deg)	99.7440(10)	90	90	93.03(3)	93.1440(10)
β (deg)	97.5900(10)	106.488(5)	105.143(2)	95.98(3)	95.9930(10)
γ(deg)	96.8580(10)	90	90	110.98(3)	110.9720(10)
Z	2	4	4	2	2
V ($Å^3$)	1354.9(3)	3719.8(7)	7453.9(7)	2350.2(9)	2350.6(4)
D_c (Mgm^{-3})	1.102	1.100	1.126	1.165	1.276
μ (mm^{-1})	0.065	0.077	0.177	1.391	1.935
F (000)	484	1328	2720	868.0	926
Reflns collected	9858	166380	336625	90050	27628
Unique reflns	4721	8597	17072	10522	10669
Parameters	313	453	823	512	475
Goodness of fit	1.006	1.072	1.025	1.062	1.025
θ range (deg)	1.32-24.99	3.101-27.616	2.933-27.563	2.981- 27.582	1.210 - 27.530
R_1 ($I > 2\sigma(I)$)	0.0491	0.0957	0.1074	0.0622	0.0361
wR_2 ($I > 2\sigma(I)$)	0.1678	0.1811	0.2898	0.1449	0.0876
R(int)	0.0214	0.1431	0.1147	0.0487	0.0425
Largest diff.peak	0.305	0.290	1.021	0.43	0.977
and hole (e. $Å^{-3}$)	-0.190	-0.797	-0.797	-0.59	-1.118

Table S2 Crystallographic data for complexes **5**, **6**, **7**, **8**

	5	**6**	**7**	**8**
Formula	$C_{43}H_{58}Cl_2N_3O_3Yb$	$C_{39}H_{56}N_3Si_2Y$	$C_{39}H_{56}ErN_3Si_2$	$C_{39}H_{56}N_3Si_2Yb$
FW	908.86	711.95	790.30	796.09
Space group	P-1	C 1 2/c 1	P-1	P-1
T (K)	298.15 K	298.15 K	298.15 K	298.15 K
Crystal system	triclinic	Monoclinic	triclinic	Triclinic
a (Å)	11.400(10)	13.872(2)	11.4267(8)	11.4008(10)
b (Å)	13.189(12)	17.623(2)	18.5276(13)	18.4999(16)
c (Å)	17.09(5)	36.834(6)	20.0773(14)	20.1152(18)
α (deg)	93.34(9)	90	93.5150(10)	93.4610(10)
β (deg)	95.90(4)	91.546(4)	98.1530(10)	98.1800(10)
γ(deg)	111.100	90	98.1800	97.8690(10)
Z	2	8	4	8
V ($Å^3$)	2372(8)	9001(2)	4150.4(5)	4146.0(6)
D_c (Mgm^{-3})	1.273	1.051	1.265	1.275
μ (mm^{-1})	2.120	1.374	2.107	2.341
F (000)	930	3024	1628	1636
Reflns collected	27749	115728	47688	47293
Unique reflns	10704	7921	18624	18538
Parameters	475	371	835	896
Goodness of fit	1.033	1.068	1.016	1.021
θ range (deg)	1.204-27.549	2.151-24.999	1.028-27.573	1.03-27.51
R_1 ($I > 2\sigma(I)$)	0.0356	0.1076	0.0314	0.0266
wR_2 ($I > 2\sigma(I)$)	0.0860	0.3165	0.0787	0.0611
R(int)	0.0395	0.1048	0.0224	0.0258
Largest diff.peak	0.787	0.955	0.930	1.136
and hole (e. $Å^{-3}$)	-1.299	-0.641	-1.552	-1.317

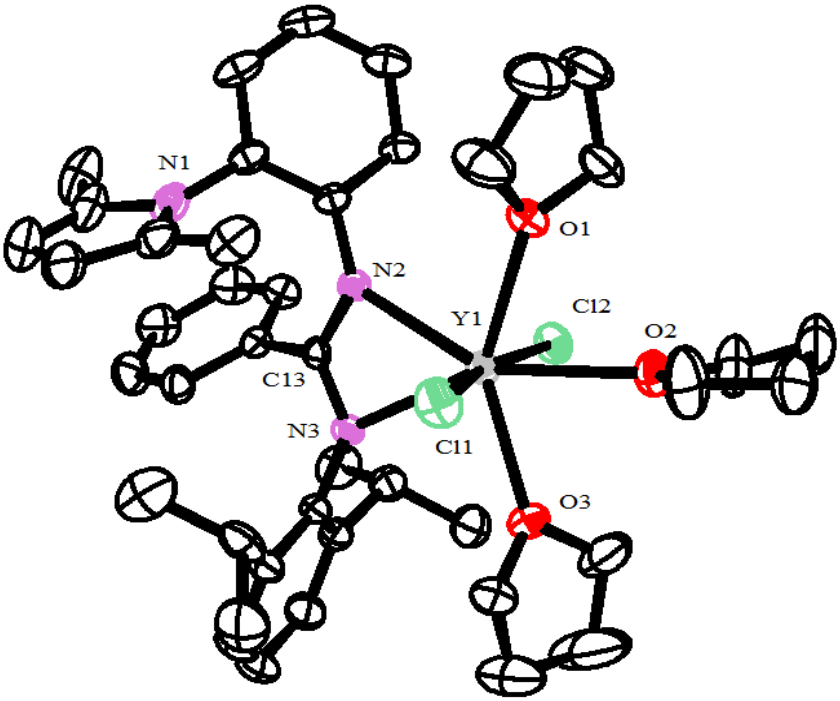

Figure S1. Molecular structure of complex **3**

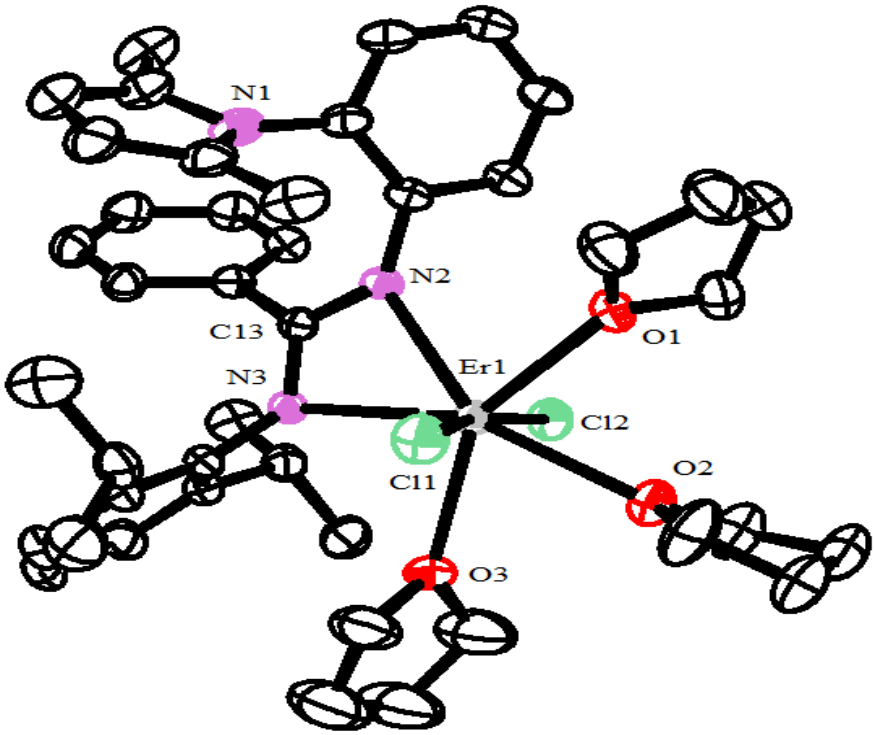

Figure S2. Molecular structure of complex **4**

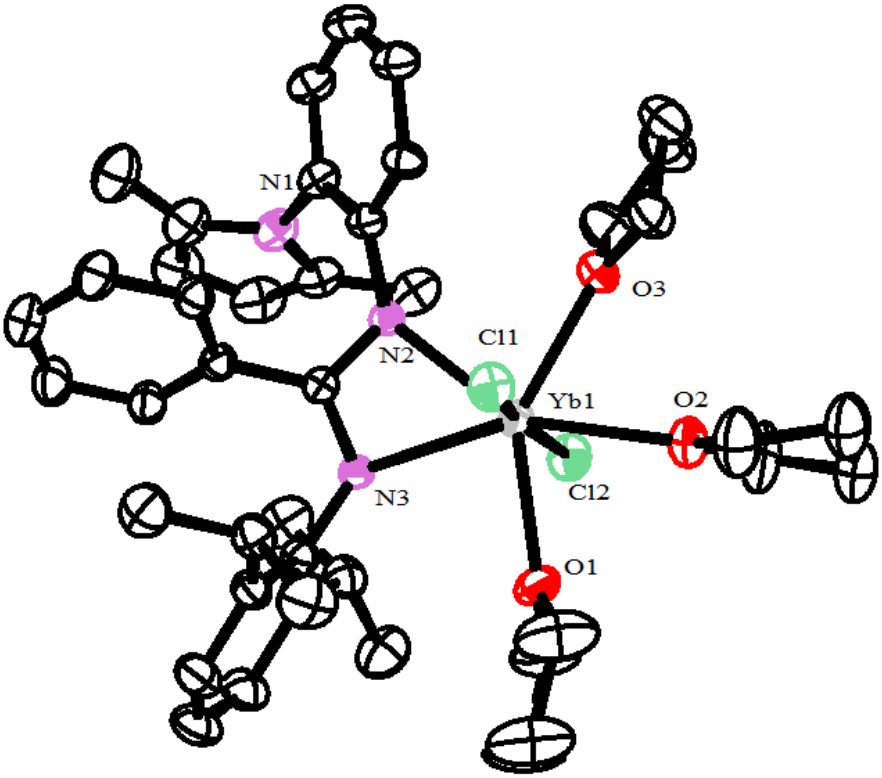

Figure S3. Molecular structure of complex **5**

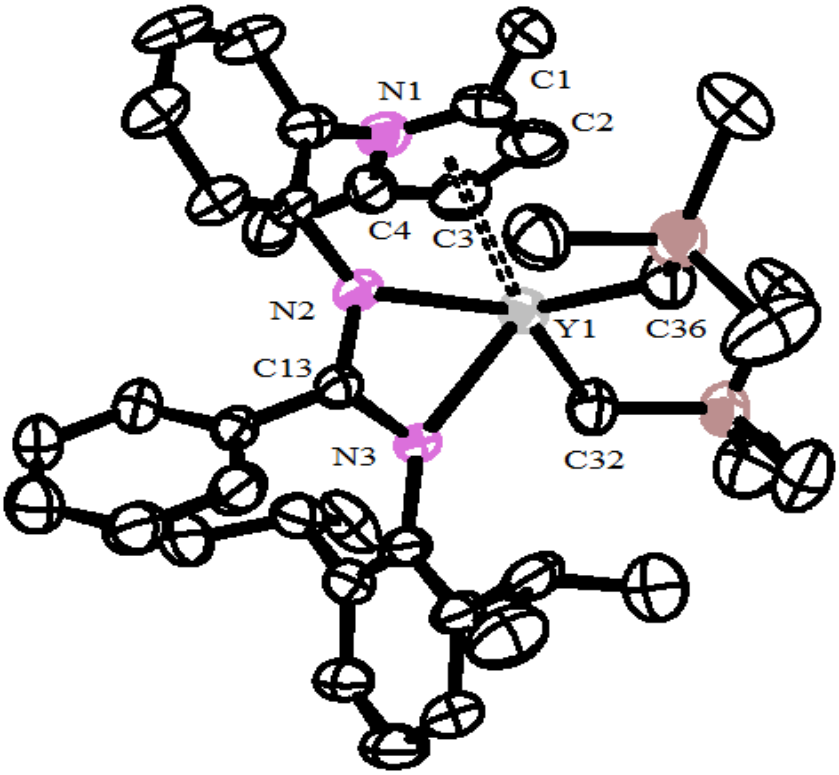

Figure S4. Molecular structure of complex **6**

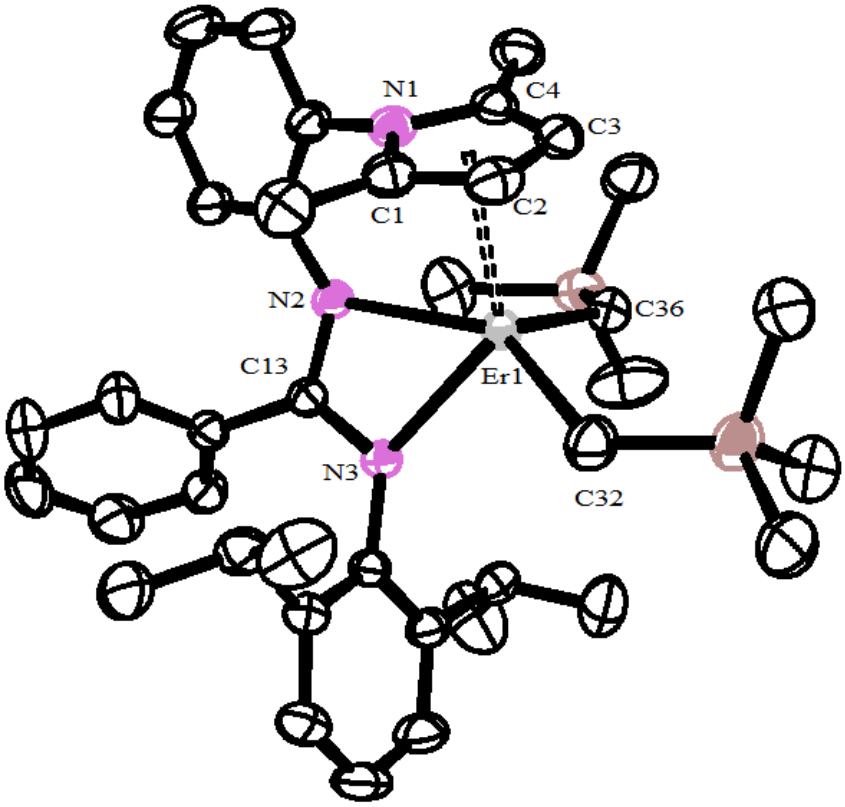

Figure S5. Molecular structure of complex **7**

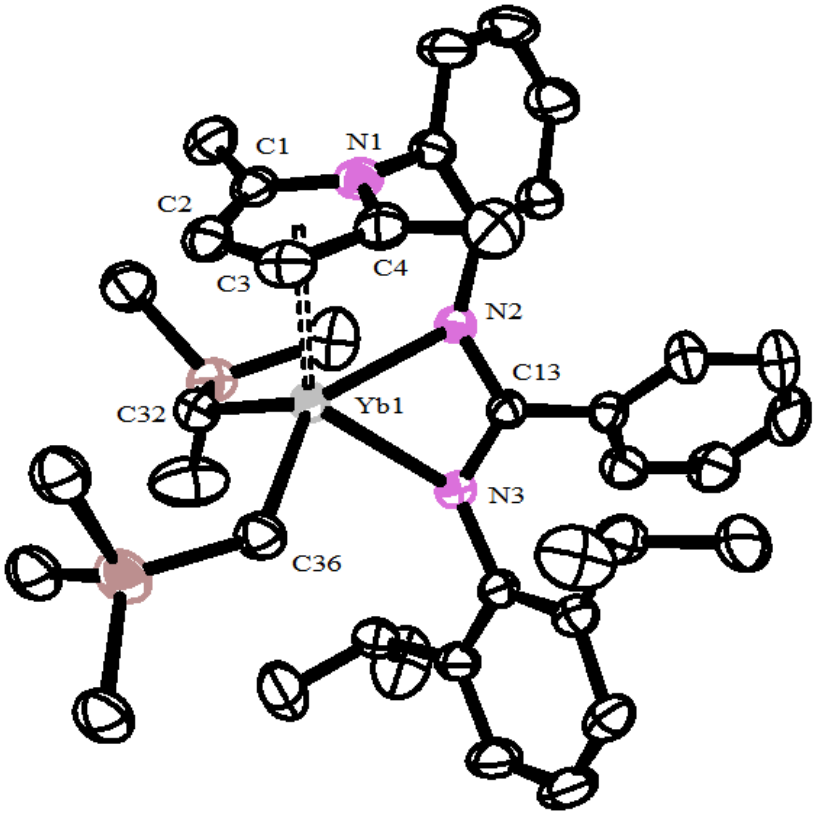

Figure S6. Molecular structure of complex **8**

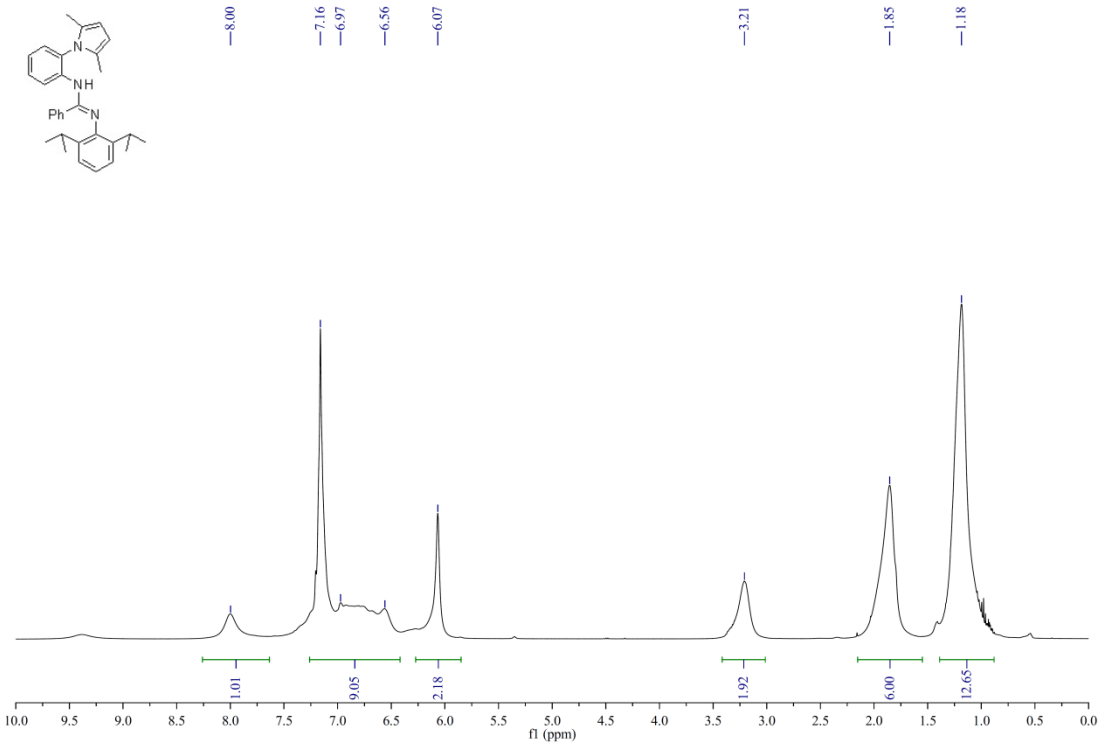

Figure S7. ^{1}H NMR spectroscopy of **HL** in C_6D_6

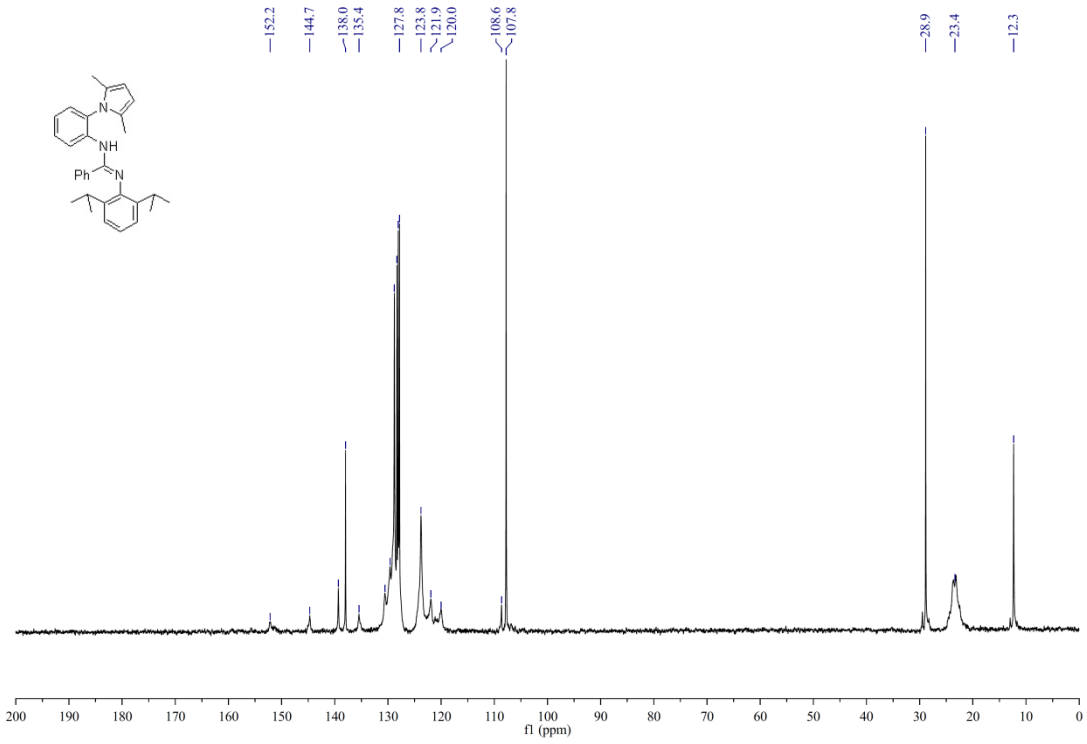

Figure S8. ^{13}C NMR spectroscopy of **HL** in C_6D_6

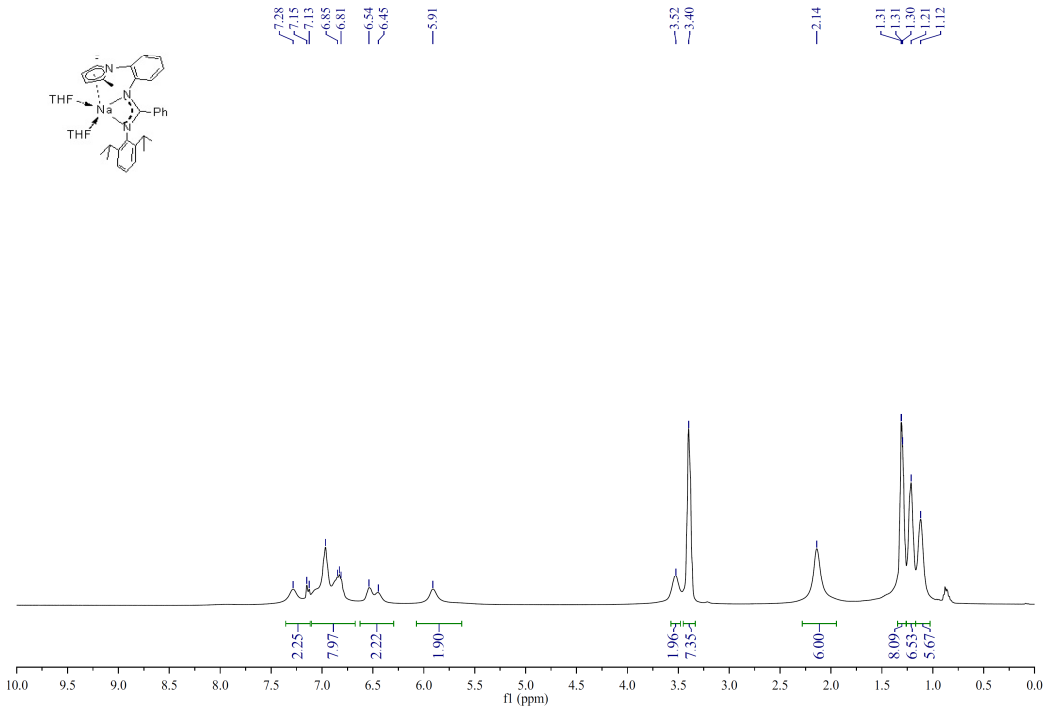

Figure S9. ^{1}H NMR spectroscopy of complex **1** in C_6D_6

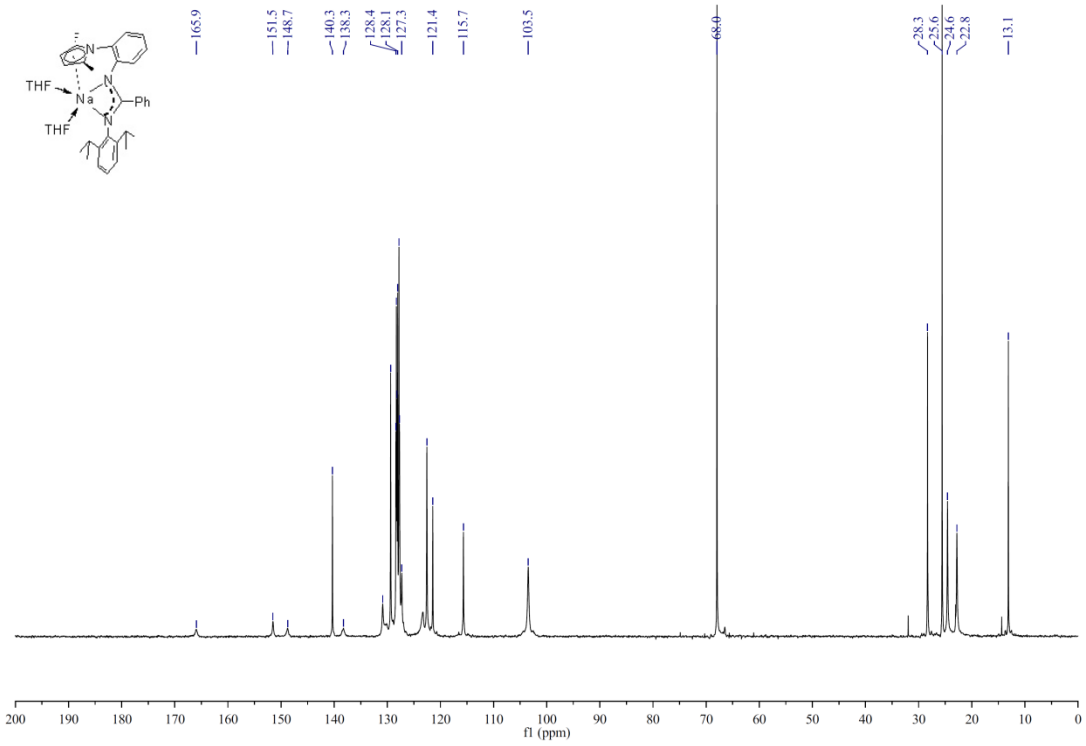

Figure S10. ^{13}C NMR spectroscopy of complex **1** in C_6D_6

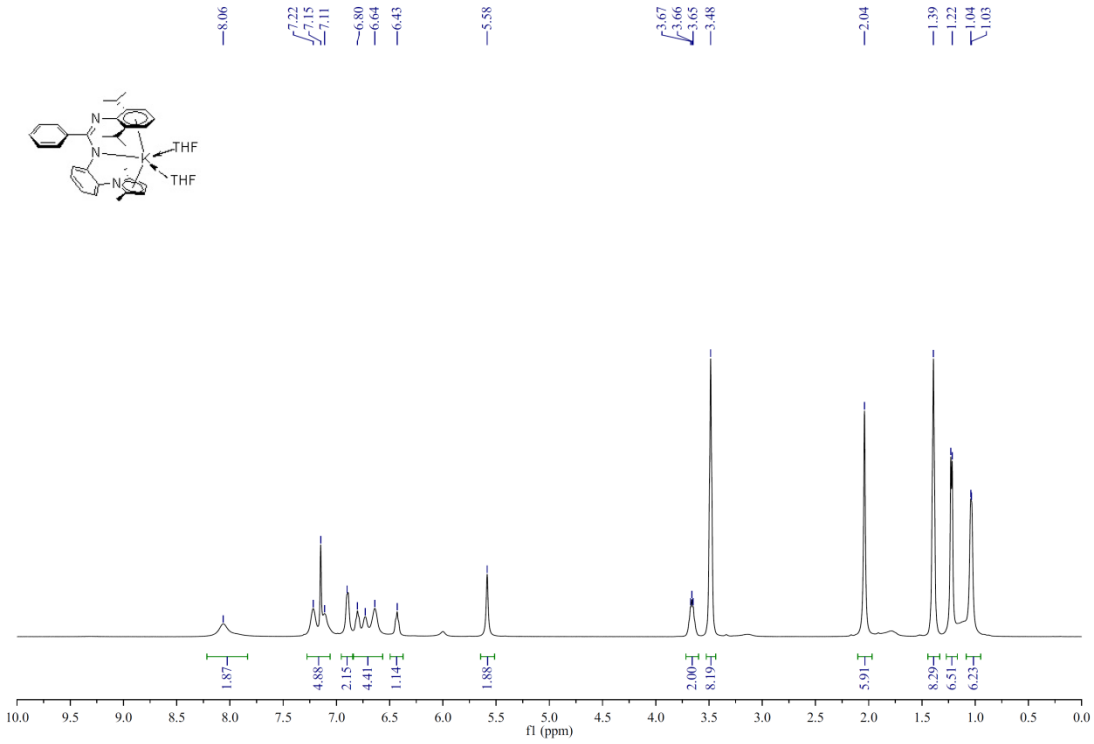

Figure S11. ^{1}H NMR spectroscopy of complex **2** in C_6D_6

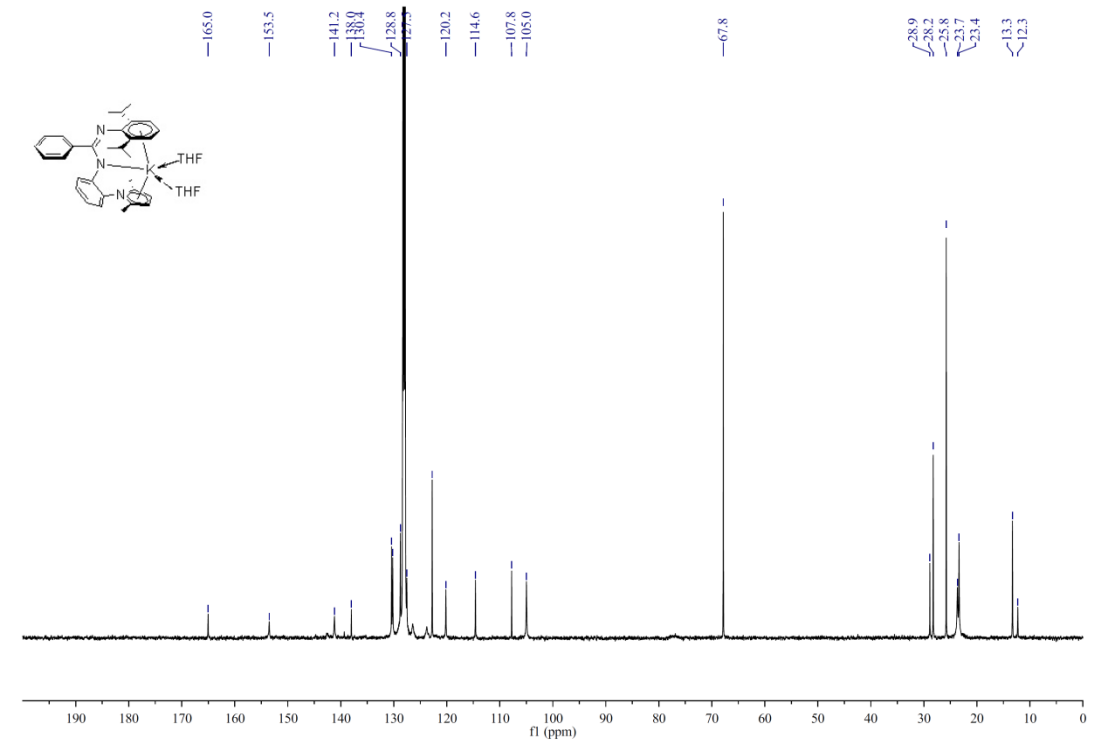

Figure S12. ^{13}C NMR spectroscopy of complex **2** in C_6D_6

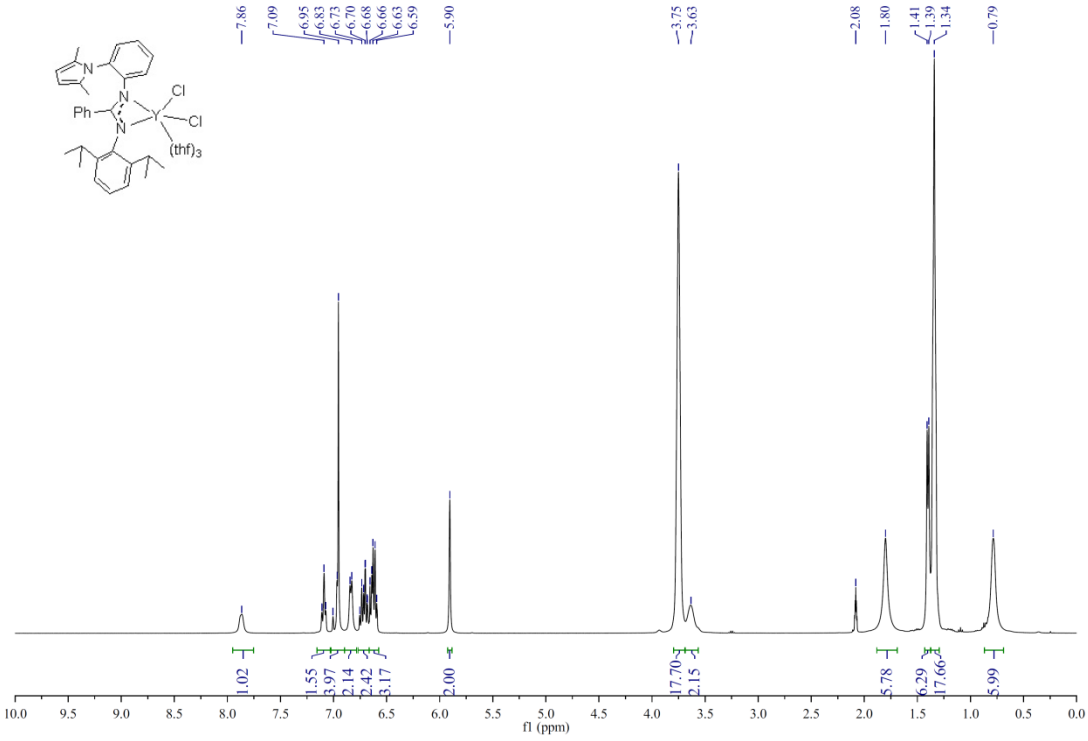

Figure S13. ^{1}H NMR spectroscopy of complex **3** in *d*8-tol

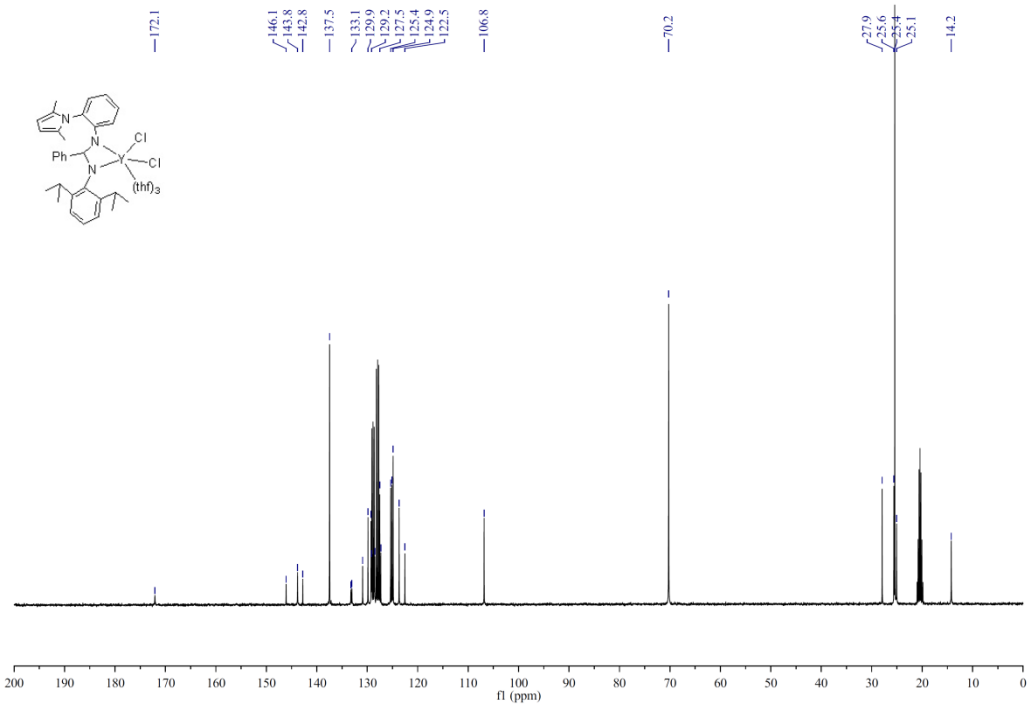

Figure S14. ^{13}C NMR spectroscopy of complex **3** in *d*8-tol

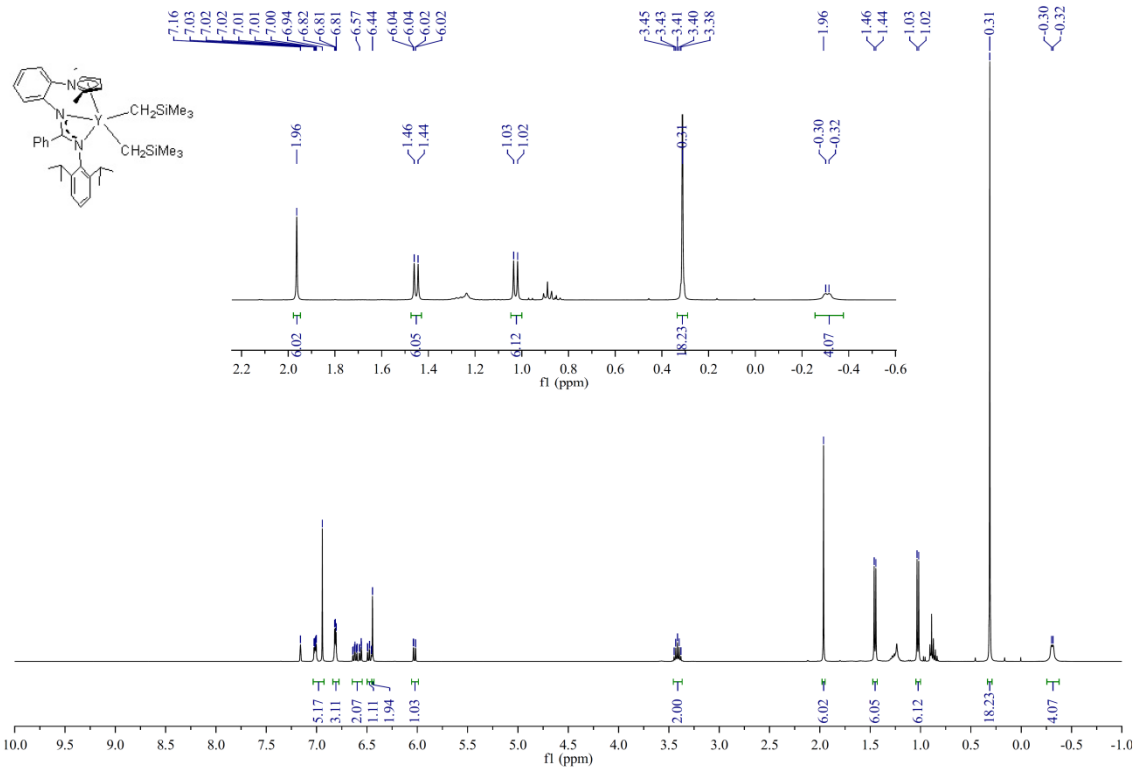

Figure S15. ^{1}H NMR spectroscopy of complex **6** in C_6D_6

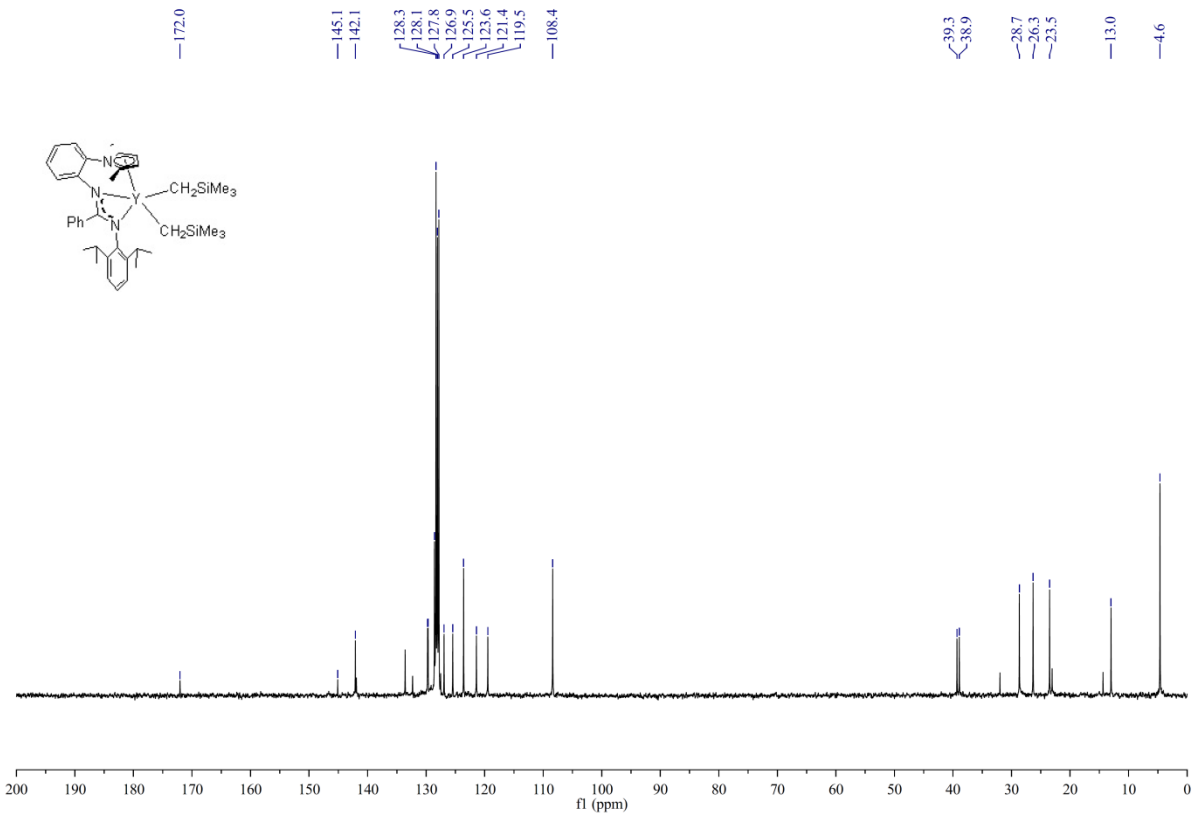

Figure S16. ^{13}C NMR spectroscopy of complex **6** in C_6D_6