Supporting information

Reactivity of Rare-earth Metal Complexes Stabilized by Anilido-Phosphinimine Ligand

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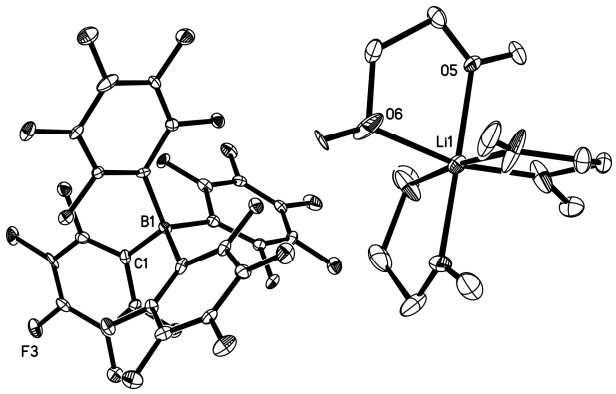
Legend

Synthesis of $[Ph_3C][B(C_6F_5)_4]$·LiCl: The powder of Ph_3CCl was added to a hexane suspension of $Li[B(C_6F_5)_4]$ at room temperature. The yellow mixture was stirred for another 6 h, and then filtrated. The isolated yellow solid was heated under vacuum for 6 h at 130 °C, to remove some undesired material as brown oil on the wall of ampoule. The residue yellow-green solids were the product $[Ph_3C][B(C_6F_5)_4]$·LiCl. We tried to remove LiCl by recrystallization $[Ph_3C][B(C_6F_5)_4]$·LiCl from dichloromethane[1] but obtained oils. Then, we repeated the reaction following the above procedure but skipped the recrystallization and obtained pure $[Ph_3C][B(C_6F_5)_4]$·LiCl. In this manuscript case the presence of LiCl didn't influence the property of this trityl salt and some other cases when it is used as an activator as compared to the LiCl-free $[PhNMe_2H][B(C_6F_5)_4]$.

[1] Chien, J. C. W.; Tsai, W. M.; Rausch, M. D. *J. Am. Chem. Soc.* **1991**, *113,* 8570



SFigure 1. Molecular structure of $[Li(DME)_3]^+[B(C_6F_5)_4]^-$ (hydrogen atoms omitted for clarity; thermal ellipsoids with 50% probability).

STable 1 Crystal data and structure refinement for **2**·($3C_6H_6$), **3**·($2C_6H_6$), **4**, **5** and **6**·DME.

	2·($3C_6H_6$)	**3**·($2C_6H_6$)	**4**	**5**	**6**·DME
Empirical formula	$C_{98}H_{106}N_4O_2P_2Y_2$	$C_{60}H_{70}N_2OPY$	$C_{43}H_{51}N_2O_2PClLu$	$C_{48}H_{60}N_2O_2PLu$	$C_{63}H_{72}N_2O_4PLu$
Formula weight	1611.61	955.06	869.25	902.92	1127.17
Crystal color	Colorless	Colorless	Colorless	Colorless	Red
Temperature (K)	187(2)	187(2)	187(2)	187(2)	187(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	P–1	P2(1)/c	P2(1)/c	P2(1)/c	P-1
a(Å)	13.7167(10)	10.1923(6)	17.1659(10)	12.3146(11)	11.8114(15)
b(Å)	13.9005(10)	35.370(2)	12.4296(7)	18.2989(17)	13.0915(16)
c(Å)	14.5758(11)	15.2058(9)	18.9236(11)	21.733(2)	20.395(3)
α(deg)	69.5510(10)	90	90	90	71.8690(10)
β(deg)	66.4810(10)	106.2860(10)	93.6180(10)	90.7990(10)	88.322(2)
γ(deg)	89.3210(10)	90	90	90	76.807(2)
Volume(Å^3)	2361.2(3)	5261.7(5)	4029.6(4)	4897.0(8)	2915.0(6)
Z	2	4	4	4	2
D_{calcd}(g/cm^3)	1.243	1.206	1.433	1.225	1.284
μ (mm^{-1})	1.309	1.179	2.593	2.083	1.767
F(000)	930	2024	1768	1856	1164
Crystal size(mm)	0.25 x 0.23 x 0.10	0.26 x 0.22 x 0.09	0.23 x 0.18 x 0.14	0.32 x 0.25 x 0.07	0.20 x 0.14x 0.08
θ range(deg)	1.58 – 26.02	1.51 – 26.06	1.96 – 26.03	1.45 – 26.04	1.68 – 26.06
Limiting indices	-16<=h<=16	-12<=h<=12	-17<=h<=21	-15<=h<=15	-10<=h<=14
	-17<=k<=16	-43<=k<=42	-15<=k<=14	-22<=k<=16	-15<=k<=16
	-16<=l<=17	-18<=l<=17	-23<=l<=23	-26<=l<=26	-25<=l<=22
Completeness to θ (%)	97.6(θ = 26.02)	99.5(θ = 26.06)	99.8(θ = 26.03)	99.8(θ = 26.04)	97.3(θ = 26.06)
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Data/restraints/parameters	9065/0/549	10381/0/621	7939/0/460	9648/110/523	11230/0/657
Goodness-of-fit on F^2	1.019	1.024	1.039	1.119	1.143
R1	0.0393	0.0517	0.0320	0.0456	0.0462
wR2	0.0952	0.1243	0.0780	0.1634	0.1402
R1 (all data)	0.0522	0.0851	0.0411	0.0585	0.0490
wR2(all data)	0.1012	0.1387	0.0826	0.1752	0.1416
Largest diff peak and hole (e Å^{-3})	0.455 and -0.225	0.814 and -0.809	1.658 and -0.721	2.013 and -0.414	3.053 and -1.211