## **Supplemental Information**

## Isolation and Characterization of Main Group and Late Transition Metal Complexes using orthoMetallated Imine Ligands

John F. Beck and Joseph A.R. Schmidt\*

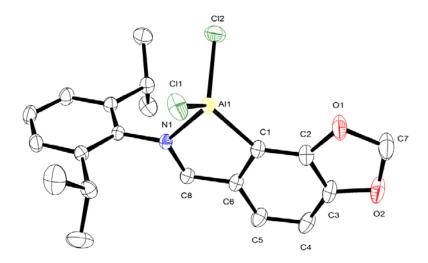
Department of Chemistry, School for Green Chemistry and Engineering, College of Natural Sciences & Mathematics, The University of Toledo

2801 W. Bancroft St. MS 602, Toledo, OH 43606-3390, USA

## **Discussion of compound 15**

The reaction of  $AlCl_3$  (1 eq.) and  $Li-L^1$  (2 eq.) yielded compound 2 in moderate yield; however, upon crystallization from toluene a single crystal of  $Al(L^1)Cl_2$  (15) was isolated. All attempts to synthesize 15 as a major reaction product failed. Changing the solvent used and the ratio of  $Li-L^1$  to  $AlCl_3$  had no effect.

**Scheme S1.** The reaction of Li-L<sup>1</sup> with AlCl<sub>3</sub> yields **2** and a small amount of **15**, which was characterized via X-ray crystallography ( $R' = 2,6^{-1}Pr_2C_6H_3$ ).



*Figure S2.* ORTEP diagram (50% thermal ellipsoids) of Al(L¹)Cl₂ (15). Hydrogen atoms removed for clarity.

 Table S1. Crystallographic data for compound 15

Compound	15
Formula	$C_{20}H_{22}AICI_2NO_2$
Formula weight	406.27
Space group	P2₁/n
Crystal system	Monoclinic
Temperature (K)	140
α (Å)	10.0807(8)
b (Å)	16.688(1)
c (Å)	12.164(1)
α (°)	90.00
β (°)	98.214(2)
γ (°)	90.00
V (ų)	2025.3(3)
Z	4
Density <sub>calc</sub> (g/cm <sup>3</sup> )	1.332
Diffractometer	Siemens SMART
Radiation	Mo- $K_{\alpha}$ ( $\lambda$ = 0.71073 Å)
Monochromator	Graphite
Detector	CCD detector
Scan type, width	ω, 0.3°
Scan speed (s)	25
Reflections measured	Hemisphere
2θ range (°)	4.18-56.66
Crystal dimensions (mm)	0.10 x 0.08 x 0.06
Reflections measured	29012
Unique reflections	5049
Observations (I > $2\sigma(I)$ )	4580
$R_{int}$	0.0358
Parameters	236
$R_{obs}$ , $R_{w}$ , $R_{all}$	0.0352, 0.0969, 0.0387
GoF	1.047

**15:** X-ray quality crystals were grown from a saturated toluene solution at -25°C. The final cycle of full-matrix least-squares refinement was based on 4580 observed reflections and 236 variable parameters and converged yielding final residuals: R = 0.0352,  $R_{all} = 0.0387$ , and GOF = 1.047.