

Bulky Guanidinato and Amidinato Zinc Complexes and their Comparative Stabilities

Cameron Jones,* Leigh Furness, Sharanappa Nembenna, Richard P. Rose, Simon Aldridge
and Andreas Stasch*

SUPPLEMENTARY MATERIAL

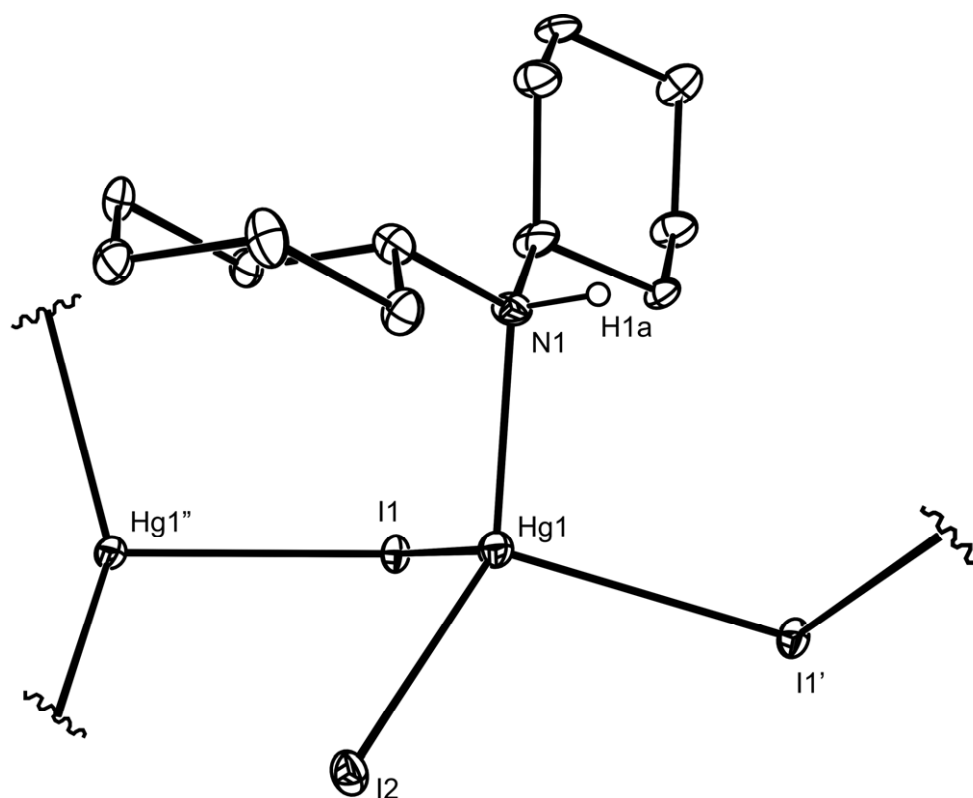


Figure S1. Molecular structure of $[\{\text{HgI}_2(\text{NCy}_2\text{H})\}]_\infty$ **1S** (25% thermal ellipsoids are shown; non-amino hydrogens omitted). Selected bond lengths (Å) and angles (°): Hg(1)-N(1) 2.276(8), Hg(1)-I(2) 2.6990(9), Hg(1)-I(1) 2.8879(11), Hg(1)-I(1') 2.8955(11), I(1)-Hg(1)'' 2.8955(11), N(1)-Hg(1)-I(2) 132.81(19), N(1)-Hg(1)-I(1) 100.9(2), I(2)-Hg(1)-I(1) 105.18(2), N(1)-Hg(1)-I(1') 102.7(2), I(2)-Hg(1)-I(1) 105.10(3), I(1)-Hg(1)-I(1') 108.83(3). Symmetry operations: ' $x, -y+1/2, z-1/2$; '' $x, -y+1/2, z+1/2$.

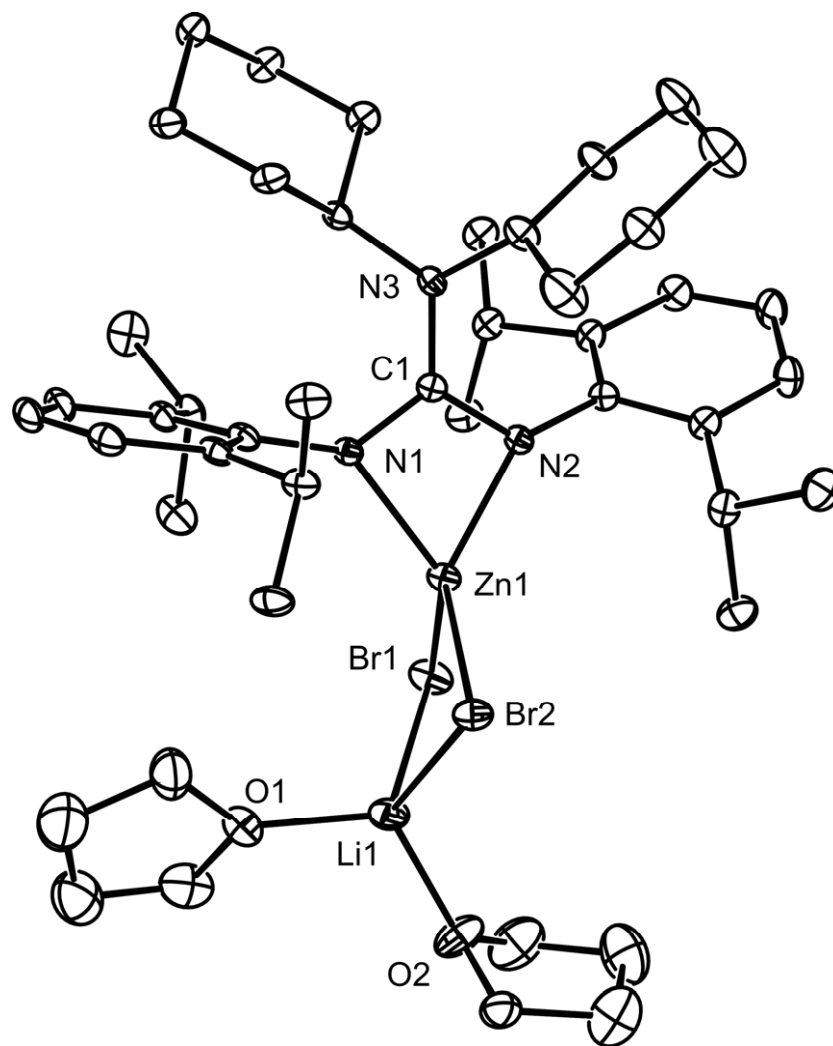


Figure S2. Molecular structure of $[(\text{Giso})\text{Zn}(\mu\text{-Br})_2\text{Li}(\text{THF})_2] \cdot 2\text{S}$ (25% thermal ellipsoids are shown; hydrogens omitted). Selected bond lengths (Å) and angles (°): Br(1)-Zn(1) 2.3879(10), Br(1)-Li(1) 2.522(12), Zn(1)-N(2) 2.012(4), Zn(1)-N(1) 2.068(4), Zn(1)-Br(2) 2.4086(11), N(1)-C(1) 1.338(7), C(1)-N(2) 1.353(7), C(1)-N(3) 1.391(7), N(2)-Zn(1)-N(1) 65.69(17), Br(1)-Zn(1)-Br(2) 101.09(4), O(2)-Li(1)-O(1) 115.0(6), Br(1)-Li(1)-Br(2) 94.0(4), N(1)-C(1)-N(2) 110.7(5).

Table S1. Crystal data for compounds [$\{\text{HgI}_2(\text{NCy}_2\text{H})\}_\infty$] **1S** and $[(\text{Giso})\text{Zn}(\mu\text{-Br})_2\text{Li}(\text{THF})_2]$ **2S**

Compound	1S	2S
Empirical Formula	$\text{C}_{12}\text{H}_{23}\text{HgI}_2\text{N}$	$\text{C}_{45}\text{H}_{72}\text{Br}_2\text{LiN}_3\text{O}_2\text{Zn}$
FW	635.70	919.19
Temp (K)	123(2)	123(2)
Cryst Syst	monoclinic	monoclinic
Space Group	$P2_1/c$	$P2_1/c$
a (Å)	10.008(2)	19.562(4)
b (Å)	17.306(4)	19.440(4)
c (Å)	9.2161(18)	12.458(3)
β (°)	96.37(3)	101.64(3)
Vol (Å ³)	1586.3(5)	4640.2(16)
Z	4	4
Density (calcd) (Mg/m ³)	2.662	1.316
$\mu(\text{Mo-K}\alpha)$ (mm ⁻¹)	13.574	2.289
F(000)	1152	1928
No. of reflections collected	7186	15390
No. of independent reflns (R_{int})	3809 (0.0595)	8093 (0.0352)
Final R1 ($I > 2\sigma(I)$) and wR2 indices (all data)	$R1 = 0.0485$ $wR2 = 0.1282$	$R1 = 0.0602$ $wR2 = 0.1663$