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Supplementary Material (6 Pages)

Preparation and Structures of Group 12 and 14 Element Halide-Carbene Complexes

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Content

Table S1. Crystallographic Experimental Details for IPr•ZnI_2

A. Crystal Data	
formula	$C_{27}H_{36}I_2N_2Zn$
formula weight	707.75
crystal dimensions (mm)	0.35 × 0.25 × 0.21
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$)
unit cell parameters[a]	
a (Å)	10.4644 (3)
b (Å)	17.4461 (5)
c (Å)	16.3027 (5)
β (deg)	98.2614 (4)
V (Å^3)	2945.38 (15)
Z	4
ρ_{calcd} (g cm^{-3})	1.596
μ (mm^{-1})	2.946
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.4°) (10 s exposures)
data collection 2θ limit (deg)	55.14
total data collected	18298 (-13 ≤ h ≤ 13, -22 ≤ k ≤ 22, -21 ≤ l ≤ 18)
independent reflections	6730 (R_{int} = 0.0150)
number of observed reflections (*NO*)	5952 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	Patterson/structure expansion (*DIRDIF–2008*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–97*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.5766–0.4271
data/restraints/parameters	6730 [$F_o^2 \geq -3\sigma(F_o^2)$] / 0 / 289
goodness-of-fit (S)[e]	1.019 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0212
wR_2 [$F_o^2 \geq -3\sigma(F_o^2)$]	0.0505
largest difference peak and hole	0.942 and –0.829 e Å^{-3}

[a]Obtained from least-squares refinement of 9961 reflections with $4.94° < 2\theta < 55.12°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Beurskens, P. T.; Beurskens, G.; de Gelder, R.; Smits, J. M. M; Garcia-Granda, S.; Gould, R. O. (2008). The *DIRDIF-2008* program system. Crystallography Laboratory, Radboud University Nijmegen, The Netherlands.

[d]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0216P)^2 + 1.8973P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

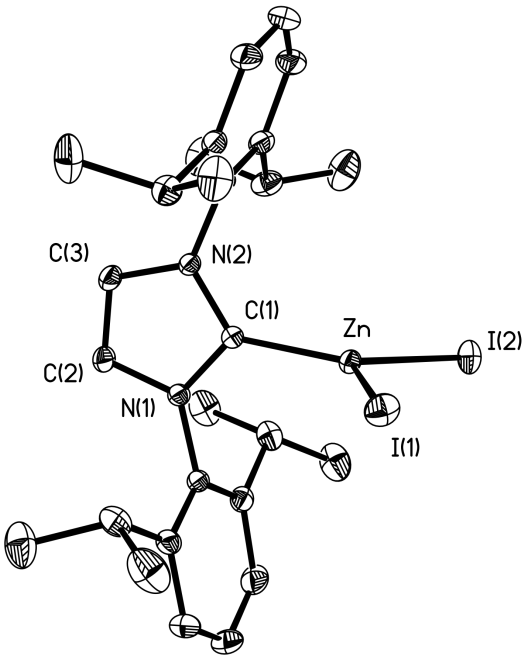
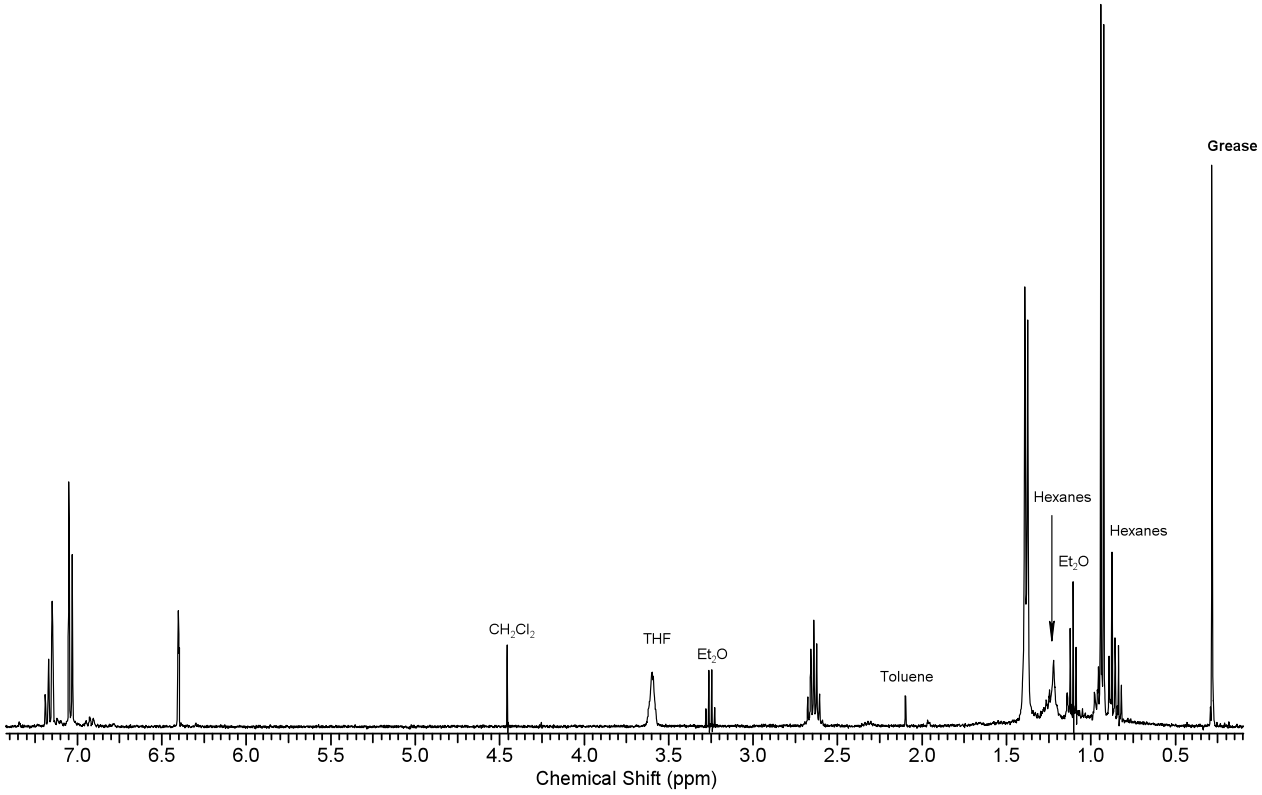


Figure S2. Thermal ellipsoid plot (30 % probability level) for IPr•ZnI_2. All hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°]: Zn-C(1) 2.0026(19), Zn-I(1) 2.5135(3), Zn-I(2) 2.5097(3); I(1)-Zn-I(2) 116.883(10), C(1)-Zn-I(1) 119.36(5), C(1)-Zn-I(2) 123.70(5); N(1)-C(1)-Zn-I(1) torsion angle = 84.45(15)°.

^{1}H NMR spectrum (in C_6D_6) of compound **7**



^{11}B NMR spectrum (in C_6D_6) of compound **7**