Electronic Supporting Information for

Donor/Acceptor Stabilization of Germanium(II) Dihydride

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Table 1. Crystallographic Experimental Details for IPr•$GeCl_2$ (**1**)

A. Crystal Data	
formula	$C_{27}H_{36}Cl_2GeN_2$
formula weight	532.07
crystal dimensions (mm)	0.28 × 0.27 × 0.05
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	10.0830 (11)
b (Å)	19.115 (2)
c (Å)	14.7562 (16)
β (deg)	99.571 (2)
V (Å^3)	2804.5 (5)
Z	4
ρ_{calcd} (g cm^{-3})	1.260
μ (mm^{-1})	1.299
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 (0.3°) (25 s exposures)
data collection 2θ limit (deg)	52.92
total data collected	10788 (-12 ≤ h ≤ 12, 0 ≤ k ≤ 23, 0 ≤ l ≤ 18)
independent reflections	10788 (R_{int} = 0.0569)
number of observed reflections (*NO*)	7693 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–97*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–97*[c])
absorption correction method	multi-scan (*TWINABS*)
range of transmission factors	0.9403–0.7140
data/restraints/parameters	10788 [$F_o^2 \geq -3\sigma(F_o^2)$] / 0 / 290
goodness-of-fit (S)[d]	1.043 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[e]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0476
wR_2 [$F_o^2 \geq -3\sigma(F_o^2)$]	0.1158
largest difference peak and hole	0.890 and –0.661 e Å^{-3}

[a]Obtained from least-squares refinement of 9891 reflections with 4.56° < 2θ < 53.94°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker. The crystal used for data collection was found to display non-merohedral twinning (twin ratio 0.68/0.32). Both components of the twin were indexed

with the program *CELL_NOW* (Bruker AXS Inc., Madison, WI, 2004). The second twin component can be related to the first component by 180º rotation about the [1 0 –1] axis in real space and about the [$-1/2$ 0 1] axis in reciprocal space. Integrated intensities for the reflections from the two components were written into a *SHELXL-93* HKLF 5 reflection file with the data integration program *SAINT* (version 7.60A), using all reflection data (exactly overlapped, partially overlapped and non-overlapped).

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

[d]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0387P)^2 + 2.4077P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

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

Table 2. Crystallographic Experimental Details for IPr•GeH_2•BH_3 (**2**)

A. Crystal Data	
formula	$C_{34}H_{49}BGeN_2$
formula weight	569.15
crystal dimensions (mm)	0.53 × 0.31 × 0.23
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	10.7242 (8)
b (Å)	16.9846 (13)
c (Å)	19.3106 (15)
α (deg)	84.4220 (10)
β (deg)	80.5350 (10)
γ (deg)	73.4210 (10)
V (Å^3)	3320.5 (4)
Z	4
ρ_{calcd} (g cm^{-3})	1.138
μ (mm^{-1})	0.945
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 (0.3°) (20 s exposures)
data collection 2θ limit (deg)	52.80
total data collected	26986 (-13 ≤ h ≤ 13, -21 ≤ k ≤ 21, 0 ≤ l ≤ 24)
independent reflections	26986 (R_{int} = 0.0271)
number of observed reflections (*NO*)	22024 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–97*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–97*[c])
absorption correction method	multi-scan (*TWINABS*)
range of transmission factors	0.8091–0.6342
data/restraints/parameters	26986 [$F_o^2 \geq -3\sigma(F_o^2)$] / 0 / 722
goodness-of-fit (*S*)[d]	1.022 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[e]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0351
wR_2 [$F_o^2 \geq -3\sigma(F_o^2)$]	0.0926
largest difference peak and hole	0.595 and –0.363 e Å^{-3}

[a]Obtained from least-squares refinement of 4042 reflections with 4.28° < 2θ < 52.84°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker. The crystal used for data collection was found to display non-merohedral twinning (twin ratio = 0.76/0.24). Both components of the twin were indexed with the program *CELL_NOW* (Bruker AXS Inc., Madison, WI, 2004). The second twin component can be related to the first component by 180° rotation about the [0.003 0 1] axis in real space and about the [0.093 0.06 1] axis in reciprocal space. Integrated intensities for the reflections from the two components were written into a *SHELXL-93* HKLF 5 reflection file with the data integration program *SAINT* (version 7.60A), using all reflection data (exactly overlapped, partially overlapped and non-overlapped).

The anisotropic displacement parameters of the solvent molecule defined by carbon atoms C20S to C26S are somewhat larger than that for the other solvent toluene (C10S to C16S). However, none of the U_{eq} values exceed 0.15 and attempts at splitting the molecule into two distinct sites led to a more poorly refining model. It is reasonable to assume that since the solvent molecules are located in a void created by the packing of the Ge complex, that there will be some degree of positional uncertainty, and/or libration, owing to the relative size of the toluene solvate molecule relative to the void volume that it occupies.

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

[d]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0435P)^2 + 0.8599P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

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

Table 3. Crystallographic Experimental Details for IPr•$SnCl_2$ (**3**)

A. Crystal Data	
formula	$C_{27}H_{36}Cl_2N_2Sn$
formula weight	578.17
crystal dimensions (mm)	0.42 × 0.17 × 0.09
crystal system	orthorhombic
space group	$P2_12_12_1$ (No. 19)
unit cell parameters[a]	
a (Å)	9.325 (2)
b (Å)	15.529 (4)
c (Å)	19.495 (4)
V (Å^3)	2823.1 (11)
Z	4
ρ_{calcd} (g cm^{-3})	1.360
μ (mm^{-1})	1.111
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	51.00
total data collected	20478 (-11 ≤ h ≤ 11, -18 ≤ k ≤ 18, -23 ≤ l ≤ 23)
independent reflections	5247 (R_{int} = 0.1245)
number of observed reflections (*NO*)	3521 [$F_o^2 \geq 2\sigma(F_o^2)$]
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	0.9115–0.6545
data/restraints/parameters	5247 [$F_o^2 \geq -3\sigma(F_o^2)$] / 0 / 289
Flack absolute structure parameter[e]	-0.08(5)
goodness-of-fit (*S*)[f]	1.066 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[g]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0596
wR_2 [$F_o^2 \geq -3\sigma(F_o^2)$]	0.1513
largest difference peak and hole	1.209 and –0.564 e Å^{-3}

[a]Obtained from least-squares refinement of 3165 reflections with 4.18° < 2θ < 33.98°.

[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]Flack, H. D. *Acta Crystallogr.* **1983**, *A39*, 876–881; Flack, H. D.; Bernardinelli, G. *Acta Crystallogr.* **1999**, *A55*, 908–915; Flack, H. D.; Bernardinelli, G. *J. Appl. Cryst.* **2000**, *33*, 1143–1148. The Flack parameter will refine to a value near zero if the structure is in the correct configuration and will refine to a value near one for the inverted configuration.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0725P)^2]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

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

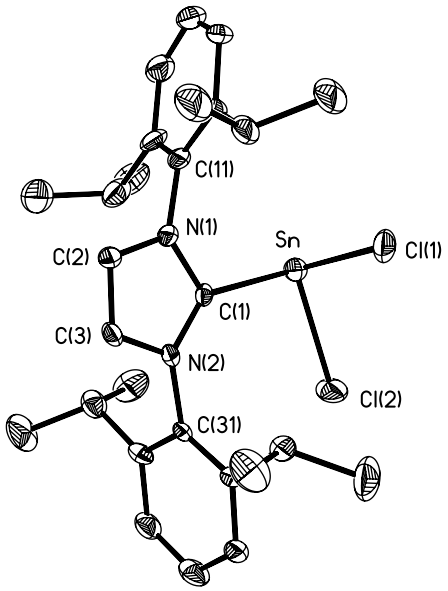

Figure S1 Thermal ellipsoid plot (30 % probability level) for IPr•$SnCl_2$ (**3**). Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Sn-Cl(1) 2.439(3), Sn-Cl(2) 2.426(2), Sn-C(1) 2.341(8); Cl(1)-Sn-Cl(2) 94.19(10), Cl(1)-Sn-C(1) 89.80(19), Cl(2)-Sn-C(1) 96.04(19), N(1)-C(1)-N(2) 110.6(6).