

Supporting Information for:

Low-coordinate germylene and stannylene heterocycles featuring sterically tunable bis(amido)silyl ligands

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2) Figure S1: Thermal ellipsoid plot (30% probability level) for $\text{Li}_2[\text{NSiN}]^{\text{Dipp}}$ *Page S-4*

Table S1. Crystallographic Experimental Details for $\text{Li}_2[\text{NSiN}]^{\text{Dipp}}$ *A. Crystal Data*

| | |
|-------------------------------------------------|----------------------------------------------------------------------------------|
| formula | C ₅₄ H ₉₆ Li ₂ N ₂ O ₆ Si |
| formula weight | 911.30 |
| crystal dimensions (mm) | 0.31 × 0.31 × 0.27 |
| crystal system | orthorhombic |
| space group | <i>P</i> 2 ₁ 2 ₁ 2 ₁ (No. 19) |
| unit cell parameters ^a | |
| <i>a</i> (Å) | 14.7015 (5) |
| <i>b</i> (Å) | 18.1668 (6) |
| <i>c</i> (Å) | 10.5297 (3) |
| <i>V</i> (Å ³) | 2812.26 (16) |
| <i>Z</i> | 2 |
| <i>ρ</i> _{calcd} (g cm ⁻³) | 1.076 |
| <i>μ</i> (mm ⁻¹) | 0.087 |

B. Data Collection and Refinement Conditions

| | |
|-------------------------------------------------------|-----------------------------------------------------------------------|
| diffractometer | Bruker D8/APEX II CCD ^b |
| radiation (λ [Å]) | graphite-monochromated Mo K α (0.71073) |
| temperature (°C) | -100 |
| scan type | ω scans (0.3°) (20 s exposures) |
| data collection 2 θ limit (deg) | 55.16 |
| total data collected | 25138 (-18 ≤ <i>h</i> ≤ 18, -23 ≤ <i>k</i> ≤ 23, -13 ≤ <i>l</i> ≤ 13) |
| independent reflections | 6490 ($R_{\text{int}} = 0.0247$) |
| number of observed reflections (<i>NO</i>) | 5559 [$F_o^2 \geq 2\sigma(F_o^2)$] |
| structure solution method | direct methods (<i>SHELXS-97</i> ^c) |
| refinement method | full-matrix least-squares on F^2 (<i>SHELXL-97</i> ^c) |
| absorption correction method | Gaussian integration (face-indexed) |
| range of transmission factors | 0.9768–0.9731 |
| data/restraints/parameters | 6490 / 0 / 303 |
| Flack absolute structure parameter ^d | 0.05(15) |
| goodness-of-fit (<i>S</i>) ^e [all data] | 1.051 |
| final <i>R</i> indices ^f | |
| <i>R</i> ₁ [$F_o^2 \geq 2\sigma(F_o^2)$] | 0.0491 |
| <i>wR</i> ₂ [all data] | 0.1470 |
| largest difference peak and hole | 0.333 and -0.167 e Å ⁻³ |

^aObtained from least-squares refinement of 9987 reflections with $4.48^\circ < 2\theta < 48.14^\circ$.

^bPrograms for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S1. Crystallographic Experimental Details (continued)

^cSheldrick, G. M. *Acta Crystallogr.* **2008**, A64, 112–122.

^dFlack, 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. In this case the relatively large standard uncertainty indicates that the structural data alone should not be used to confirm absolute stereochemistry, but should be used in conjunction with the established stereochemistry of the precursor compound.

^e $S = [Sw(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0816P)^2 + 0.5281P]^{-1}$ where $P = [\text{Max}(F_o^2, 0) + 2F_c^2]/3$).

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

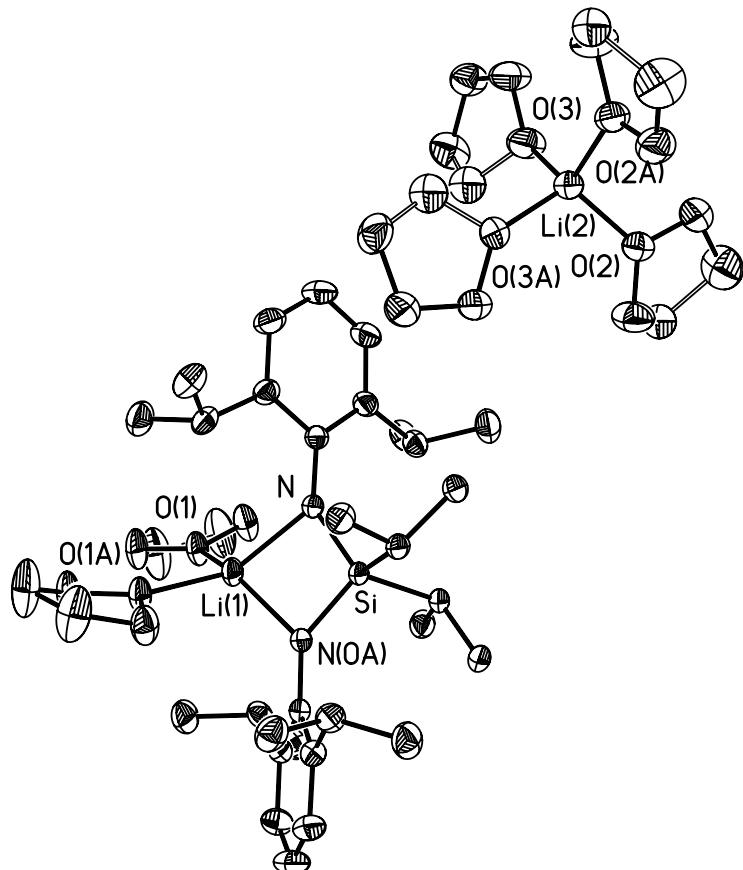


Figure S1. Molecular structure of $\text{Li}_2[\text{NSiN}]^{\text{Dipp}}$ [$\{(\text{DippN})_2\text{Si}^{\text{i}}\text{Pr}_2\}\text{Li}(\text{THF})_2\}[\text{Li}(\text{THF})_4]$ with thermal ellipsoids at the 30 % probability level. All hydrogen atoms omitted for clarity. Primed atoms related to unprimed ones by the 2-fold axis at $(1/2, 0, 0)$. Selected bond lengths (\AA) and angles ($^{\circ}$): Si(1)-N(1) 1.6971(15), Si(1)-C(1) 1.92257(19), N(1)-Li(1) 2.038(3), Li(1)-O(1) 2.038(3), Li(2)-O(2) 1.924(4), Li(2)-O(3) 1.901(4).