

Supporting Information

Unexpected Formation and Structural Characterization of a Dinuclear Sodium Half-Sandwich Complex

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Crystal data and details on structure refinement of $[\text{NaC}_5\text{H}_3\{\text{C}(\text{NH}^i\text{Pr})(=\text{N}^i\text{Pr})\}_2-1,2]_2$ (**1**).

Crystallographer: P. Liebing

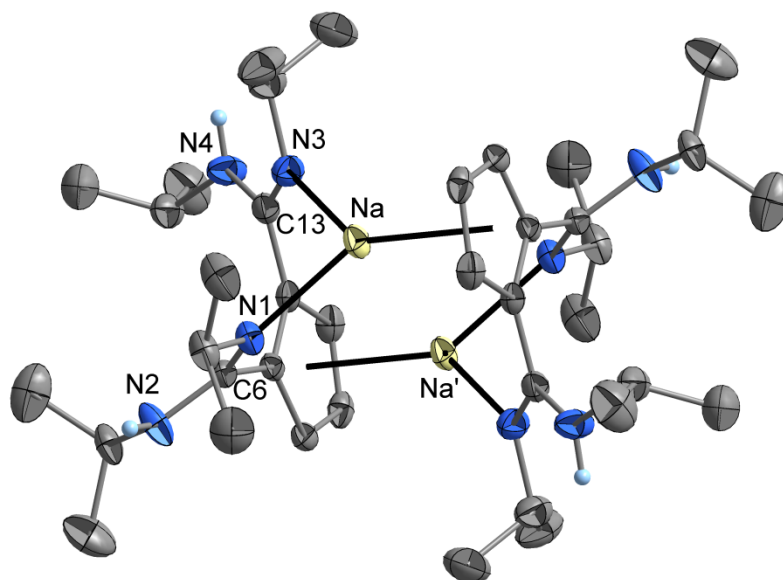


Figure S1. Molecular structure of $[\text{NaC}_5\text{H}_3\{\text{C}(\text{NH}^i\text{Pr})(=\text{N}^i\text{Pr})\}_2-1,2]_2$ (**1**) in the crystal. Displacement ellipsoids are drawn at the 50% probability level, H atoms attached to C atoms omitted for clarity. Symmetry code: $'-x, -y, 2-z$.

formula sum	$\text{C}_{38}\text{H}_{66}\text{N}_8\text{Na}_2$
formula weight	680.96
crystal color/shape/size (mm)	colorless prisms / $0.54 \times 0.32 \times 0.15$
crystal system	monoclinic
space group	$P2_1/n$
unit cell parameters	
<i>a</i> (Å)	10.293(2)
<i>b</i> (Å)	16.512(3)
<i>c</i> (Å)	12.607(3)
<i>α</i> (deg)	90
<i>β</i> (deg)	101.73(3)
<i>γ</i> (deg)	90
unit cell volume <i>V</i> (Å ³)	2097.9(8)
molecules per cell <i>z</i>	2
crystallographic density ρ_{calcd} (g cm ⁻³)	1.078
absorption coefficient μ (mm ⁻¹)	0.083

diffractometer	STOE IPDS 2T
radiation (λ [Å])	graphite-monochromated Mo-K $_{\alpha}$ (0.71073)
temperature (°C)	−120(2)
scan type	ω scan
completeness of dataset	99.8%
θ range of data collection (deg)	2.368 ... 25.999
reflections collected	11527 ($-12 \leq h \leq 11$, $-20 \leq k \leq 19$, $-15 \leq l \leq 15$)
independent reflections	4108 ($R_{\text{int}} = 0.0284$)
independent reflections with $I > 2\sigma(I)$	3166
structure solution method	direct methods (ShelXS-97)
refinement method	full-matrix least-squares on F^2 (SHELXL 2016/4)
absorption correction method	none
data / parameters / restraints	4108 / 233 / 0
goodness of fit (GooF) [all data]	1.023
final R values	
R_1 [all data, $I \geq 2\sigma(I)$]	0.0643, 0.0448
wR_2 [all data, $I \geq 2\sigma(I)$]	0.1158, 0.1085
largest difference peak and hole	0.233 and −0.180 e Å $^{-3}$

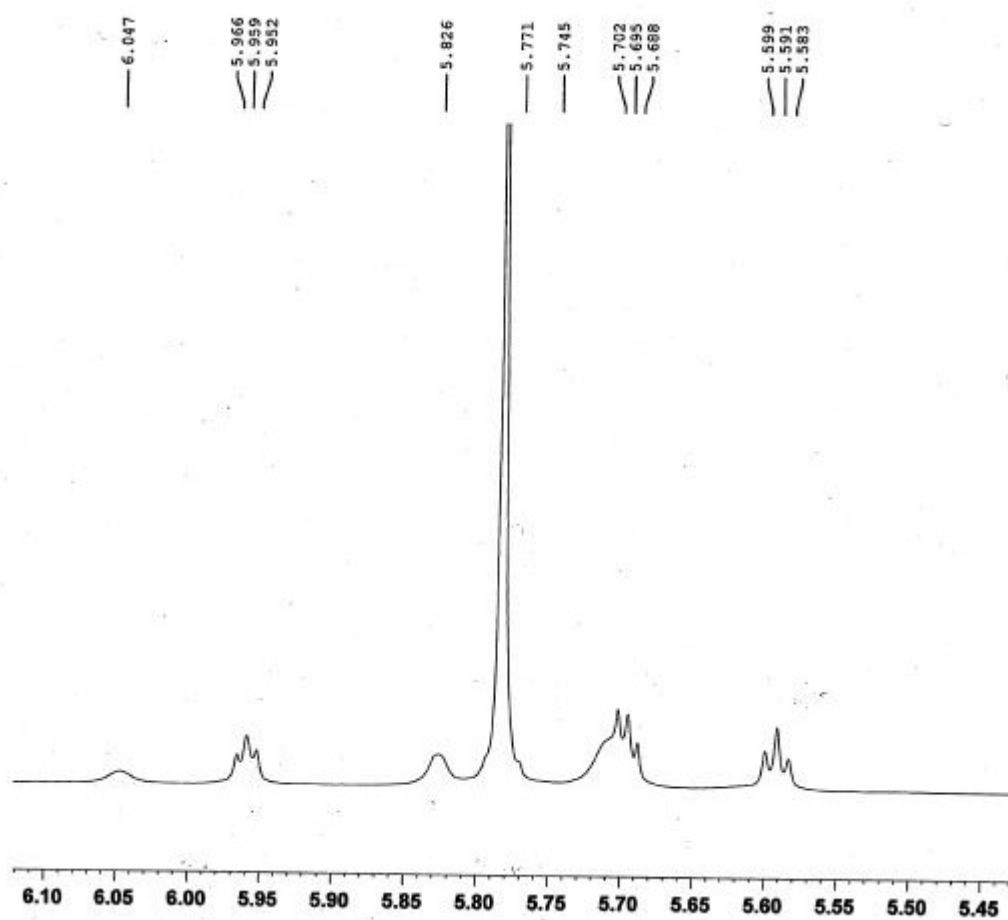


Figure S2. ^1H NMR spectrum of **1** (Part 1) in $\text{THF-}d_8$

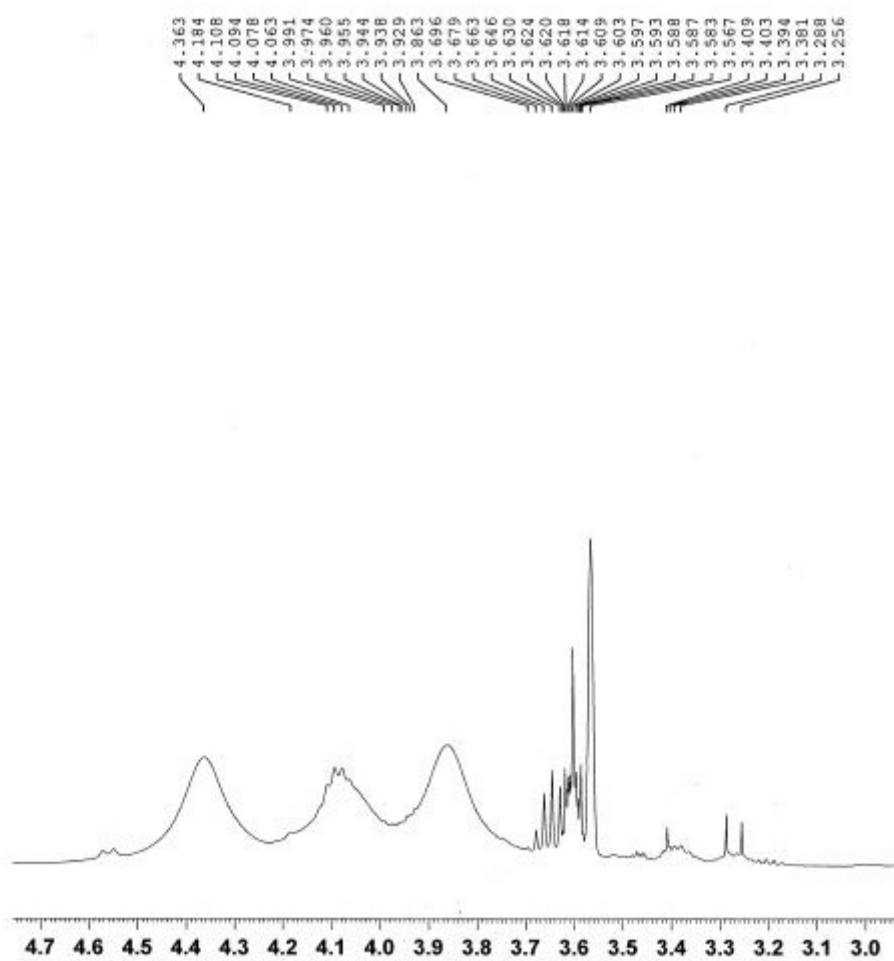


Figure S3. ^1H NMR spectrum of **1** (Part 2) in $\text{THF-}d_8$

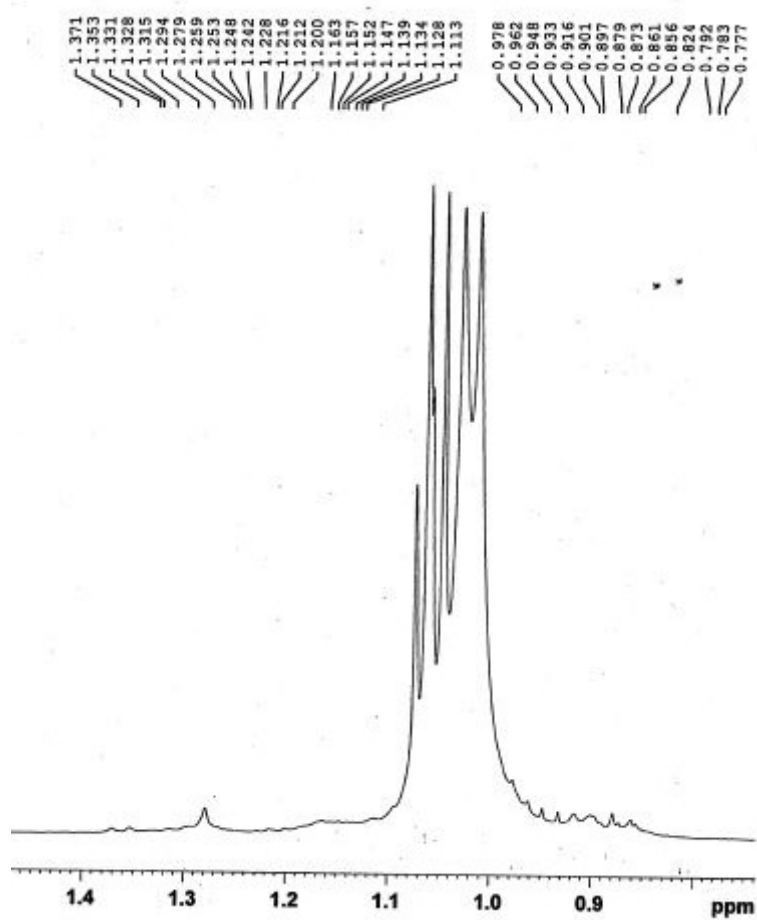


Figure S4. ^1H NMR spectrum of **1** (Part 3) in $\text{THF-}d_8$

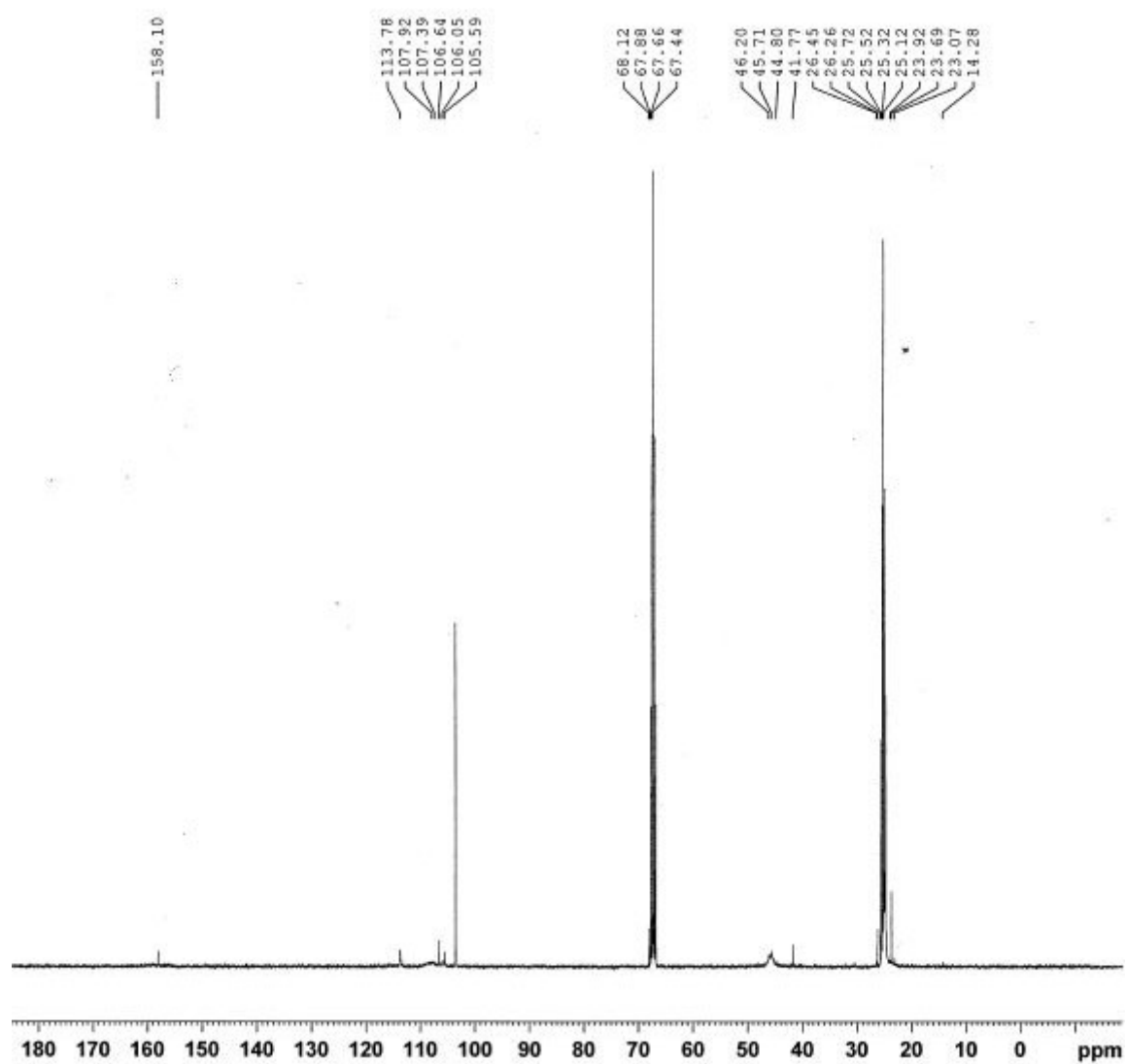


Figure S5. ^{13}C NMR spectrum of **1** in $\text{THF-}d_8$

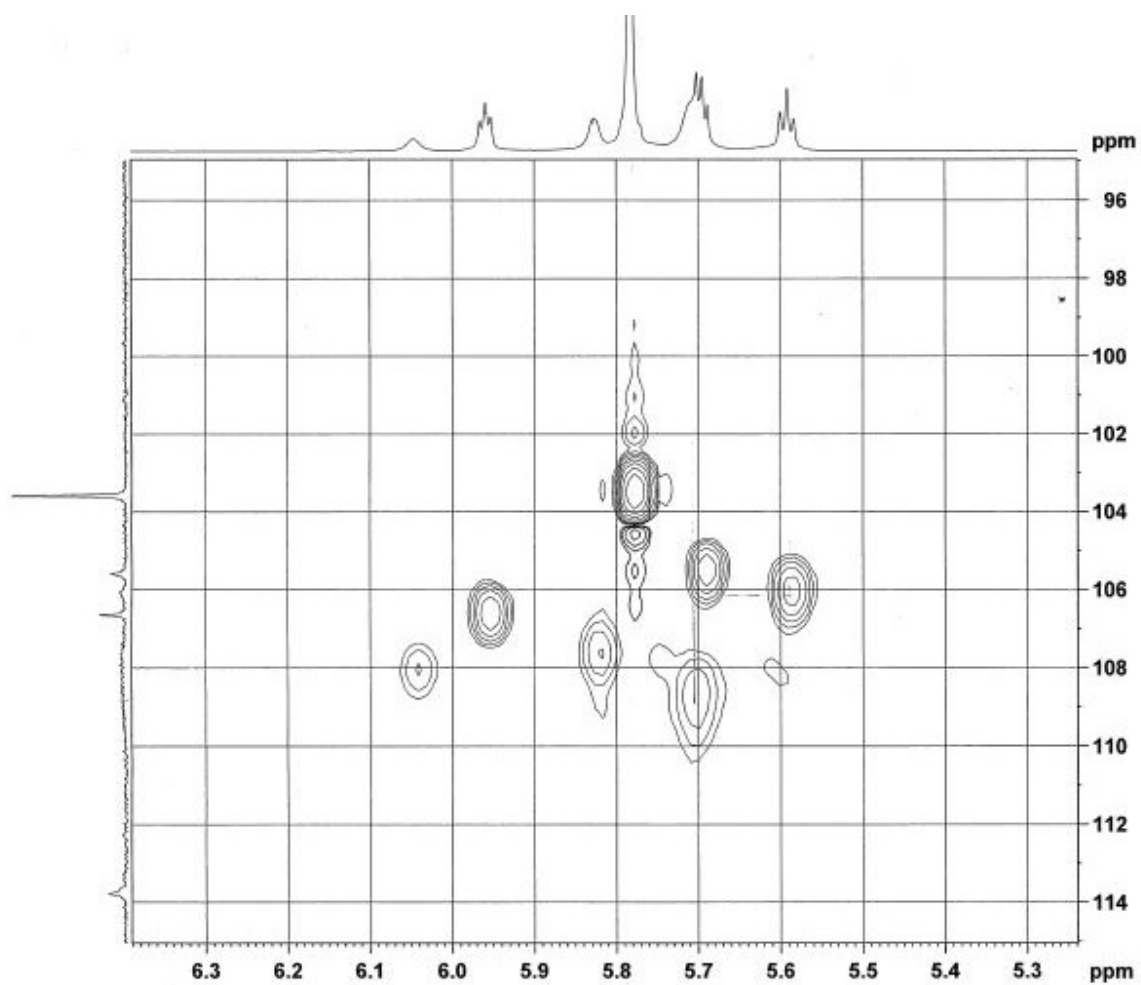


Figure S6. ^1H , ^{13}C HSQC NMR spectrum of **1** (Part 1)