

Supplementary Information

for

**Synthesis and Structures of Bimetallic and Polymeric Zinc
Coordination Compounds Supported by Salicylaldiminato and
Anilido-alimine Ligands**

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X-ray crystallography

Crystal data for 2b: $C_{38}H_{60}N_2O_2Zn_2$, $M = 707.62$, orthorhombic, $Aba2$ (no. 41), $a = 18.1320(8)$, $b = 18.8215(7)$, $c = 23.1100(9)$ Å, $V = 7886.8(5)$ Å³, $Z = 8$, $D_c = 1.192$ g cm⁻³, $\mu(\text{Mo-K}\alpha) = 1.248$ mm⁻¹, $T = 173$ K, pale yellow plates, Oxford Diffraction Xcalibur 3 diffractometer; 12497 independent measured reflections, F^2 refinement, $R_1 = 0.063$, $wR_2 = 0.149$, 11979 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{\text{max}} = 65^\circ$], 404 parameters. The structure of **1** was shown to be a partial polar twin by a combination of R -factor tests [$R_1^+ = 0.0646$, $R_1^- = 0.0726$] and by use of the Flack parameter [$x^+ = +0.260(12)$, $x^- = +0.740(12)$]. CCDC 621015.

Crystal data for 4c: $C_{45}H_{60}N_4Zn_2$, $M = 787.71$, triclinic, $P\bar{1}$ (no. 2), $a = 8.9147(5)$, $b = 14.7627(9)$, $c = 16.4967(9)$ Å, $\alpha = 88.863(6)$, $\beta = 86.406(4)$, $\gamma = 72.948(5)^\circ$, $V = 2071.5(2)$ Å³, $Z = 2$, $D_c = 1.263$ g cm⁻³, $\mu(\text{Cu-K}\alpha) = 1.676$ mm⁻¹, $T = 173$ K, yellow blocks, Oxford Diffraction Xcalibur PX Ultra diffractometer; 7684 independent measured reflections, F^2 refinement, $R_1 = 0.042$, $wR_2 = 0.120$, 6428 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{\text{max}} = 142^\circ$], 469 parameters. CCDC 621016.

The C(37) ethyl ligand in the structure of **2b**, and the C(27) isopropyl moiety in the structure of **4c**, were both found to be disordered. In each case two orientations for the terminal methyl groups were identified with *ca.* 75% and 25% occupancy, respectively; the carbon atom(s) of major occupancy orientations were refined anisotropically, whilst those of the minor occupancy orientations were refined isotropically.

Crystal data for 5c: $C_{48}H_{66}N_4Zn_2$, $M = 829.79$, monoclinic, $P2_1/n$ (no. 14), $a = 11.5694(6)$, $b = 13.4841(8)$, $c = 14.3159(7)$ Å, $\beta = 98.626(4)^\circ$, $V = 2208.1(2)$ Å³, $Z = 2$ [C_i symmetry], $D_c = 1.248$ g cm⁻³, $\mu(\text{Mo-K}\alpha) = 1.122$ mm⁻¹, $T = 173$ K, yellow blocks, Oxford Diffraction Xcalibur 3 diffractometer; 7658 independent measured reflections, F^2 refinement, $R_1 = 0.045$, $wR_2 = 0.095$, 3959 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{\text{max}} = 65^\circ$], 244 parameters. CCDC 621017.

Table S1. Selected bond lengths (Å) and angles (°) for **5c**.

Zn–N(1)	1.9277(16)	Zn–N(7)	1.9906(17)
Zn–C(23)	1.947(2)		
N(1)–Zn–N(7)	94.65(7)	N(1)–Zn–C(23)	139.00(9)
N(7)–Zn–C(23)	126.34(9)		

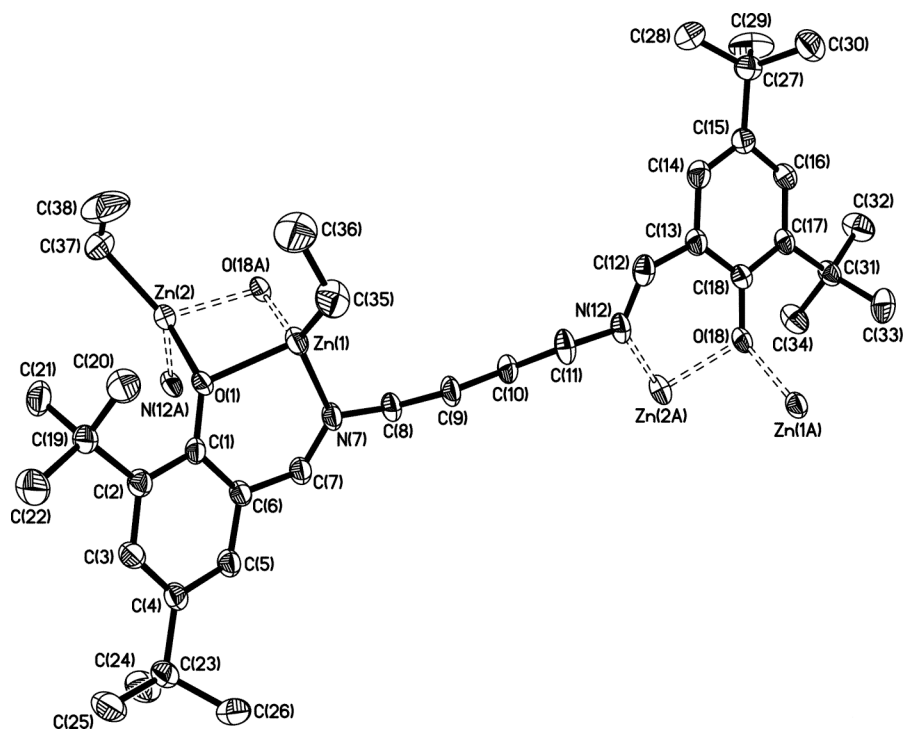


Fig. S1 The asymmetric unit in the structure of **2b** (50% probability ellipsoids).

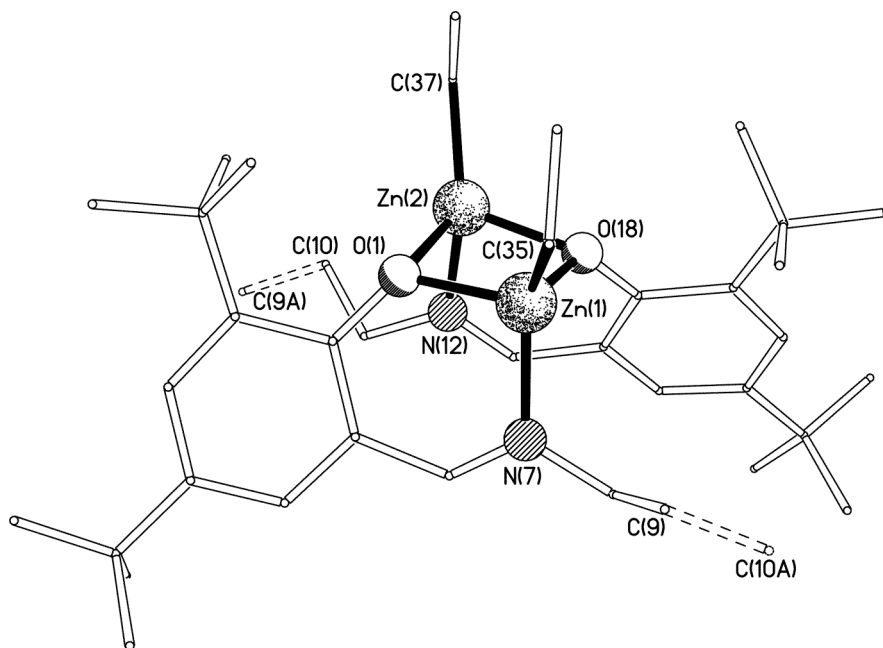


Fig. S2 The environment of the Zn_2O_2 ring in the structure of **2b**.

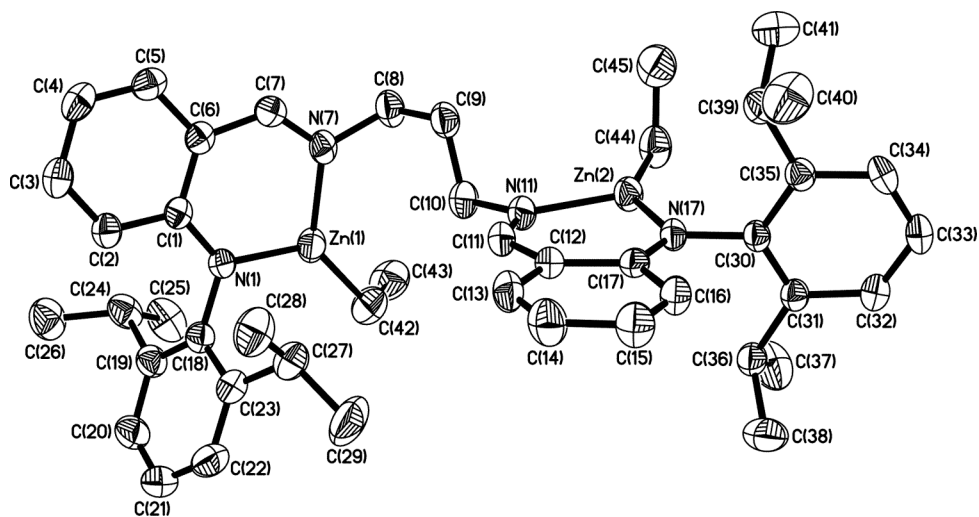


Fig. S3 The molecular structure of **4c** (50% probability ellipsoids).

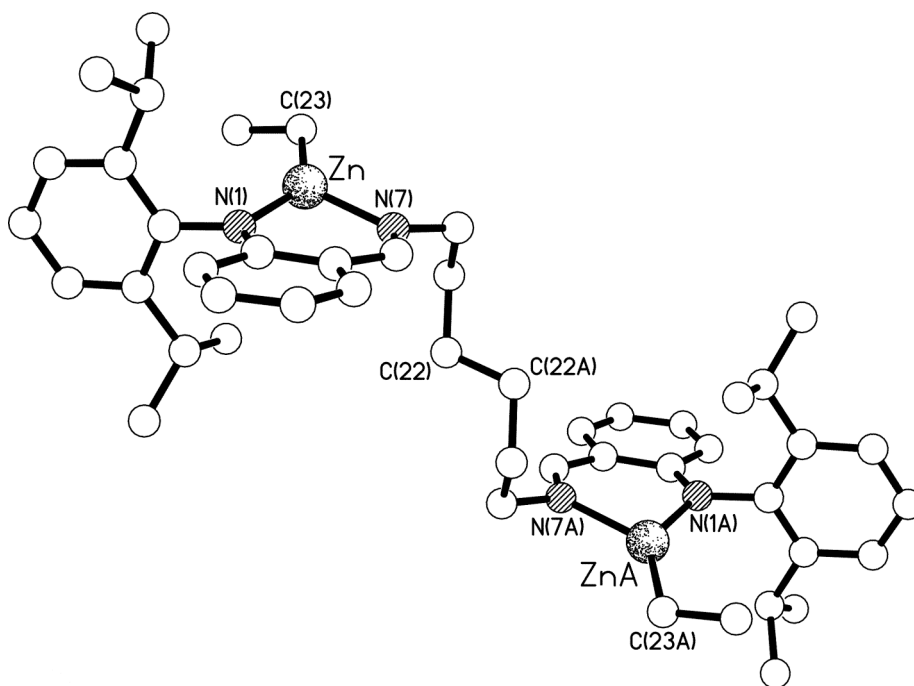


Fig. S4 The molecular structure of **5c**.

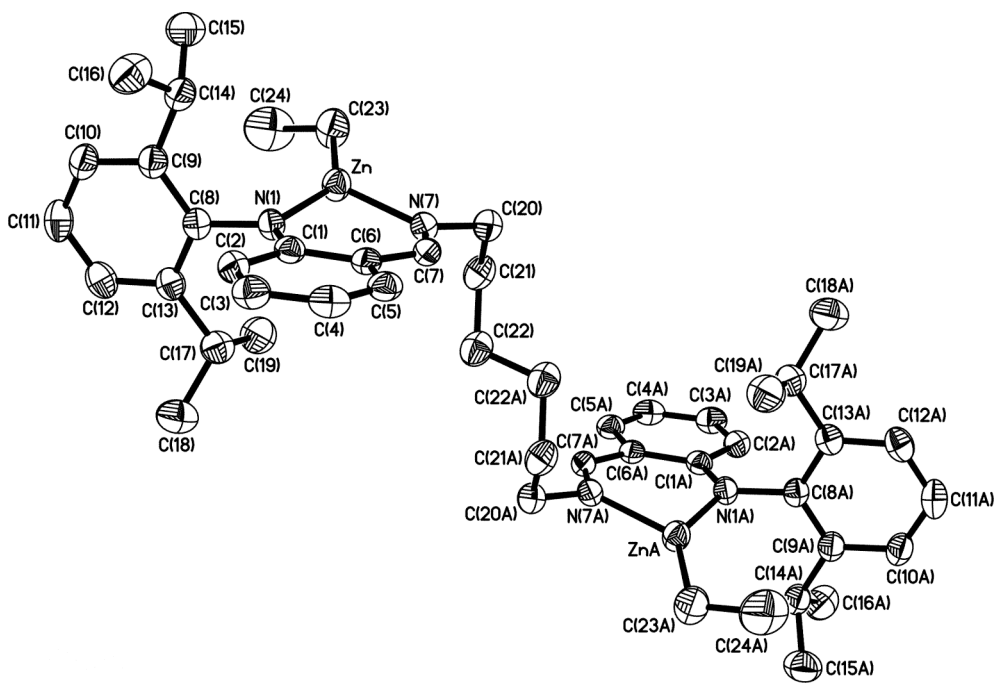


Fig. S5 The molecular structure of 5c (50% probability ellipsoids).