Supplementary Information

for

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

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X-ray crystallography

Crystal data for 2b: C_{38}H_{60}N_{2}O_{2}Zn_{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 \text{ 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°\], 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_{4}Zn_{2}, M = 787.71, triclinic, \(\overline{P1}\) (no. 2), a = 8.9147(5), b = 14.7627(9), c = 16.4967(9) Å, \(\alpha = 88.863(6), \beta = 86.406(4), \gamma = 72.948(5)°\), V = 2071.5(2) Å³, Z = 2, D_{c} = 1.263 g cm⁻³, \(\mu\text{(Cu-K\(\alpha\)}) = 1.676 \text{ 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°\], 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_{4}Zn_{2}, M = 829.79, monoclinic, \(P2_{1}/n\) (no. 14), a = 11.5694(6), b = 13.4841(8), c = 14.3159(7) Å, \(\beta = 98.626(4)°\), \(\gamma = 126.34(9)°\), V = 2208.1(2) Å³, Z = 2 \([\text{C}_{i} \text{ symmetry}]\), D_{c} = 1.248 g cm⁻³, \(\mu\text{(Mo-K\(\alpha\)}) = 1.122 \text{ 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°\], 244 parameters. CCDC 621017.

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

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<tr>
<td>Zn–N(1)</td>
<td>1.9277(16)</td>
<td>Zn–N(7)</td>
<td>1.9906(17)</td>
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<tr>
<td>Zn–C(23)</td>
<td>1.947(2)</td>
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<tr>
<td>N(1)–Zn–N(7)</td>
<td>94.65(7)</td>
<td>N(1)–Zn–C(23)</td>
<td>139.00(9)</td>
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<tr>
<td>N(7)–Zn–C(23)</td>
<td>126.34(9)</td>
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**Fig. S1** The asymmetric unit in the structure of 2b (50% probability ellipsoids).

**Fig. S2** The environment of the Zn$_2$O$_2$ 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).