ESI to accompany:

Environmental control in the assembly of metallomacrocycles and one-dimensional polymers with 4,2':6':4''-terpyridine linkers and zinc(II) nodes

Edwin C. Constable,[a] Catherine E. Housecroft,*[a] Alessandro Prescimone,[a] Srboljub Vujovic[a] and Jennifer A. Zampese

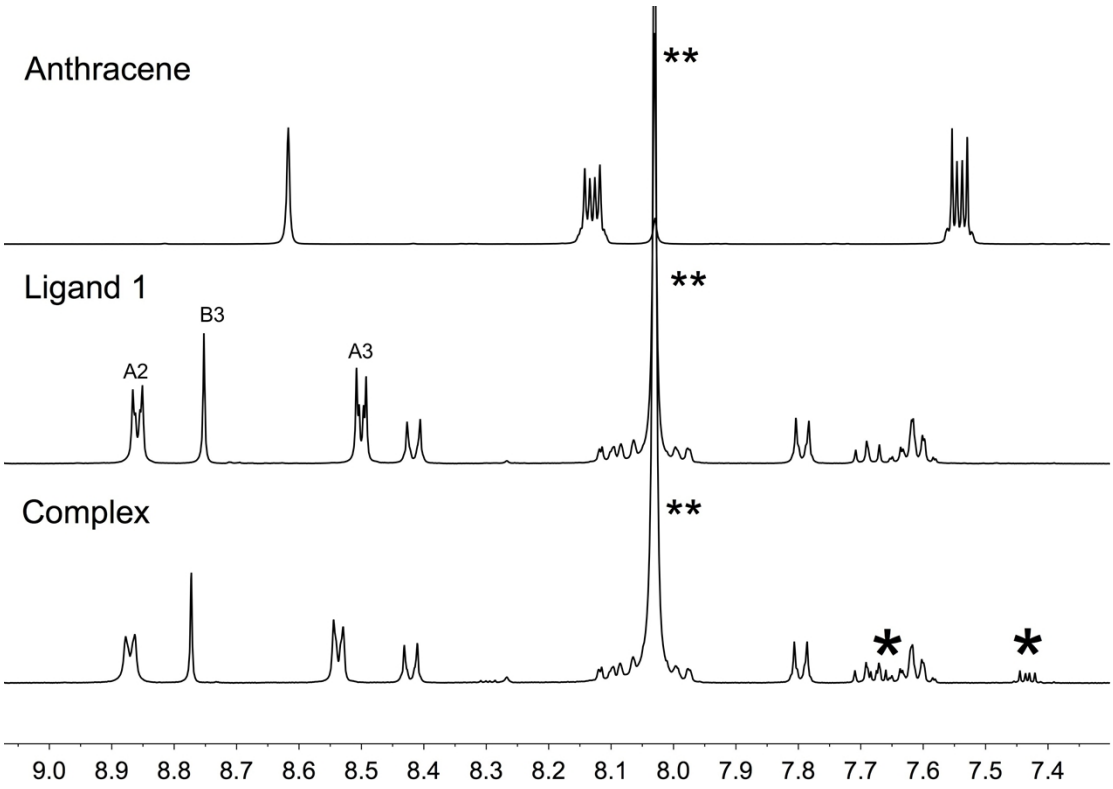

Fig. S1 400 MHz ^{1}H NMR spectra of DMF-d_7 solutions of anthracene, **1** and [{$ZnCl_2$(**1**)}$_6$]-A. ** = residual DMF; * = 1,2-$C_6H_4Cl_2$. Chemical shifts in ∂ / ppm. See Scheme 1 for atom labelling.

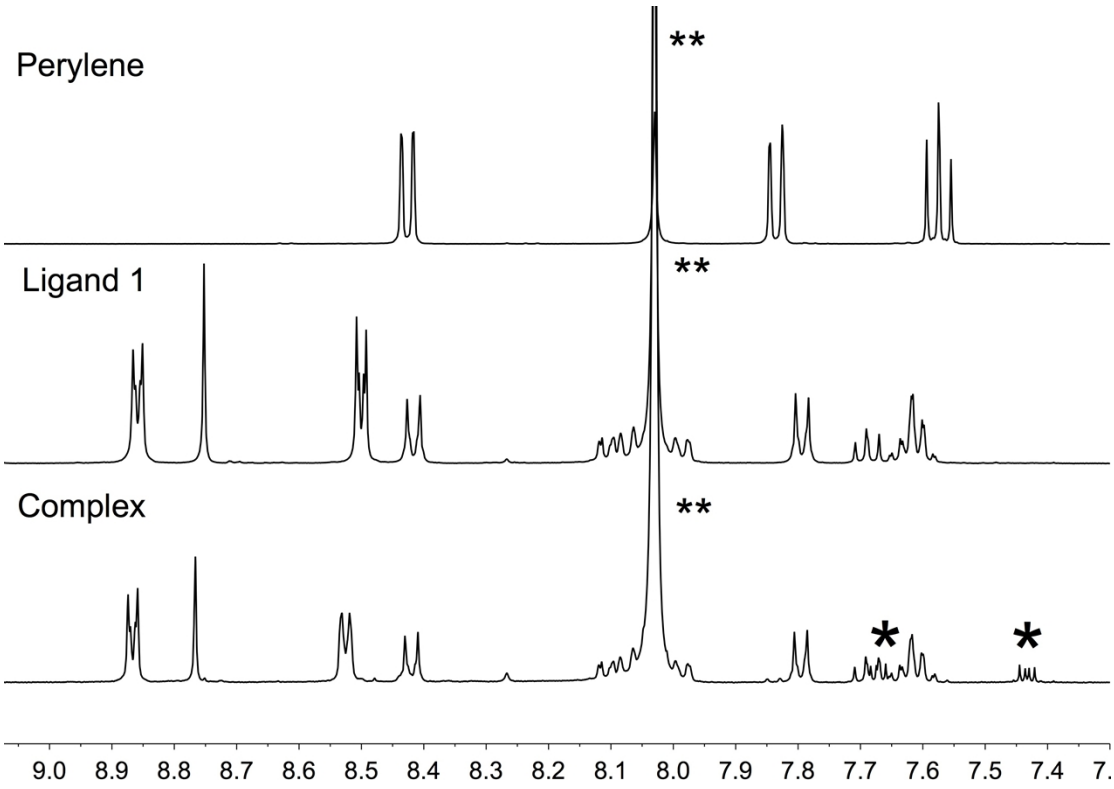

Fig. S2 400 MHz ^{1}H NMR spectra of DMF-d_7 solutions of perylene, **1** and [{$ZnCl_2$(**1**)}$_6$]-P. ** = residual DMF; * = 1,2-$C_6H_4Cl_2$. Chemical shifts in ∂ / ppm.

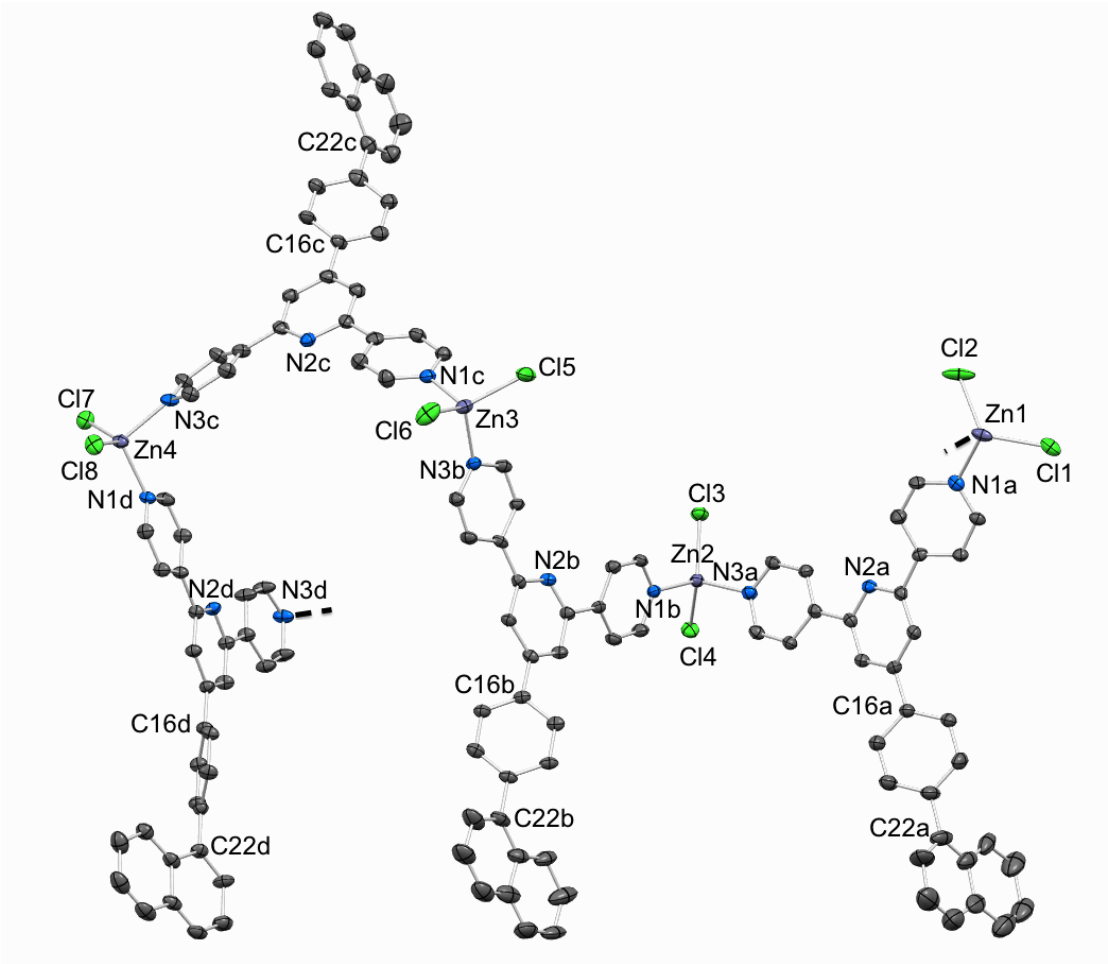

Fig. S3 ORTEP diagram of the asymmetric unit in $[ZnCl_2(\mathbf{1})]_n$ (ellipsoids plotted at 30% probability level and H atoms omitted for clarity). Selected bond lengths: Zn1–N1a = 2.049(3), Zn1–N3d^{i} = 2.069(3), Zn1–Cl2 = 2.1952(14), Zn1–Cl1 = 2.2303(15), Zn2–N1b = 2.026(3), Zn2–N3a = 2.061(3), Zn2–Cl3 = 2.2065(11), Zn2–Cl4 = 2.2354(11), Zn3–N1c = 2.028(4), Zn3–N3b = 2.062(3), Zn3–Cl6 = 2.2056(16), Zn3–Cl5 = 2.2279(15), Zn4–N3c = 2.063(4), Zn4–N1d = 2.071(3), Zn4–Cl8 = 2.1964(12), Zn4–Cl7 = 2.2140(13) Å. Symmetry code i = *x*, *y*, 1+*z*.

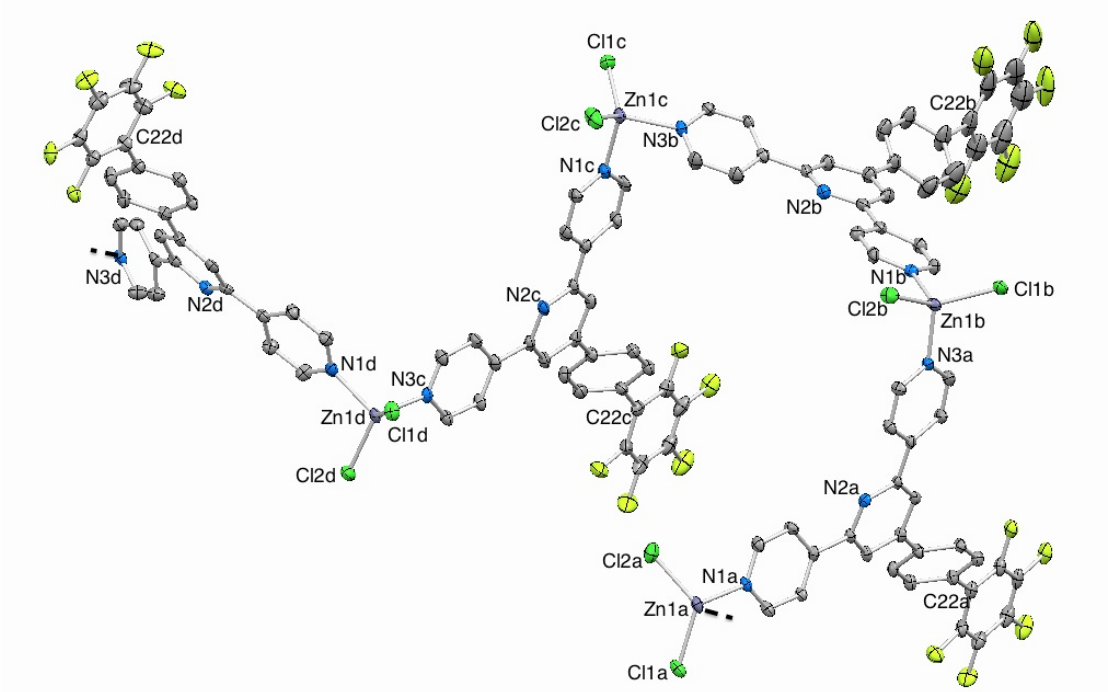

Fig. S4 ORTEP diagram of the asymmetric unit in $[ZnCl_2(\mathbf{2})]_n$ (ellipsoids plotted at 30% probability level and H atoms omitted for clarity). Selected bond lengths: Zn1A–N1a = 2.043(3), Zn1a^{i}–N3d = 2.068(4), Zn1a–Cl1a = 2.2133(14), Zn1a–Cl2a = 2.2221(16), N3a–Zn1b = 2.057(4), Zn1b–N1b = 2.068(4), Zn1b–Cl2b = 2.2125(13), Zn1b–Cl1b = 2.2187(13), N3b–Zn1c = 2.038(4), Zn1c–N1c = 2.076(4), Zn1c–Cl2c = 2.2114(15), Zn1c–Cl1c = 2.2115(14), N3c–Zn1d = 2.052(3), Zn1d–N1d = 2.077(4), Zn1d–Cl2d = 2.2049(14), Zn1d–Cl1d = 2.2082(14) Å. Symmetry code i = x, y, –1 + z.

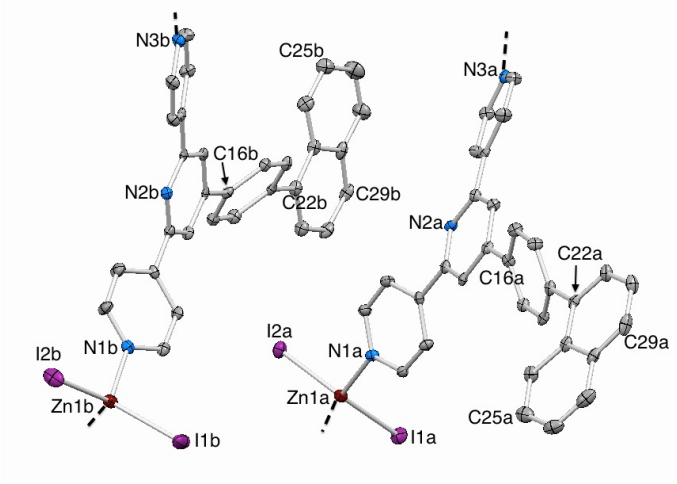

Fig. S5 ORTEP diagram of the two independent $\{ZnI_2(\mathbf{1})\}$ units in the asymmetric unit in $[2\{ZnI_2(\mathbf{1})\}\cdot CHCl_3]_n$ (ellipsoids plotted at 40% probability level and H atoms omitted for clarity). Selected bond lengths: Zn1a–N1a = 2.045(6), Zn1a–N3a^{i} = 2.053(6), Zn1a–I1a = 2.5473(9), Zn1a–I2a = 2.5576(9), Zn1b–N1b = 2.048(6), Zn1b–N3b^{ii} = 2.070(6), Zn1b–I1b = 2.5476(10), Zn1b–I2b = 2.5623(10) Å. Symmetry codes i = x, $^{1}/_{2}-y$, $-^{1}/_{2}+z$; ii = x, $^{3}/_{2}-y$, $-^{1}/_{2}+z$.