ESI to accompany:

Metallohexacycles containing 4'-aryl-4,2':6',4"-terpyridines: conformational preferences and fullerene capture

Edwin C. Constable,* Catherine E. Housecroft,* Srboljub Vujovic and Jennifer A. Zampese

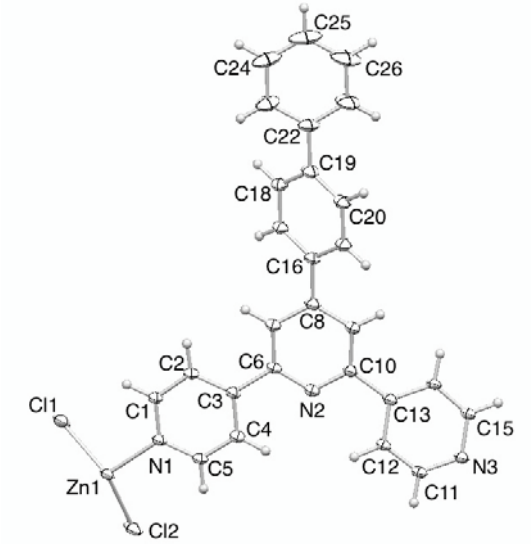

Fig. S1 ORTEP plot with atom labelling for the contents of the asymmetric unit in $[\{ZnCl_2(\mathbf{1})\}_6]\cdot 6CHCl_3\cdot 6MeOH\cdot 5H_2O$. Ellipsoids plotted at 40% probability level; solvent molecules omitted.

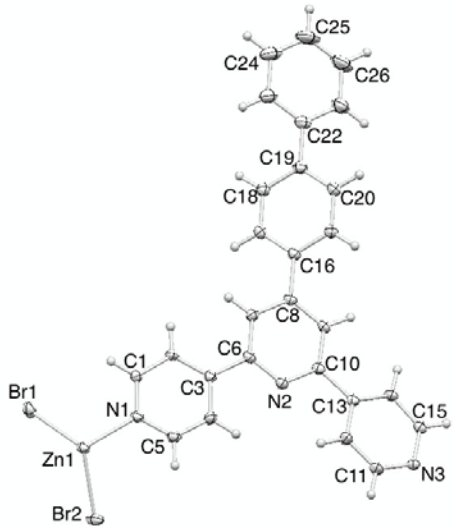

Fig. S2 ORTEP plot with atom labelling for the contents of the asymmetric unit in $[\{ZnBr_2(\mathbf{1})\}_6]\cdot 4CHCl_3\cdot 5MeOH\cdot 8H_2O$. Ellipsoids plotted at 40% probability level; solvent molecules omitted.

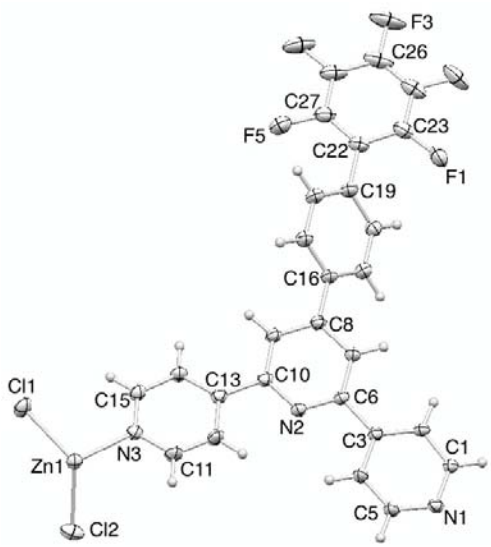

Fig. S3 ORTEP plot with atom labelling for the contents of the asymmetric unit in $[\{ZnCl_2(\mathbf{2})\}_6]\cdot 3CHCl_3\cdot 3MeOH\cdot 6H_2O$. Ellipsoids plotted at 40% probability level; solvent molecules omitted

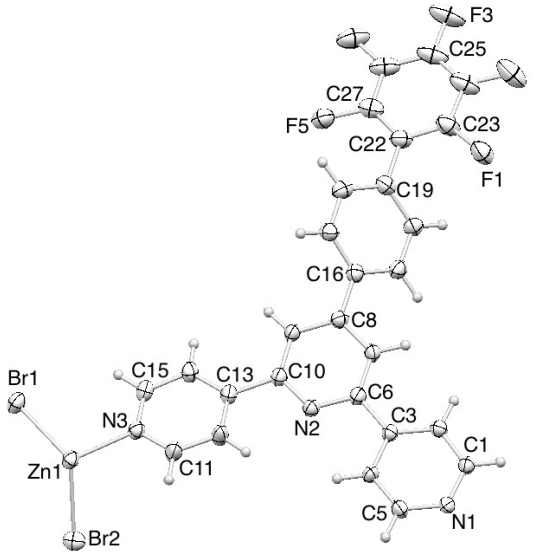

Fig. S4 ORTEP plot with atom labelling for the contents of the asymmetric unit in $[\{ZnBr_2(\mathbf{2})\}_6]$. Ellipsoids plotted at 30% probability level.

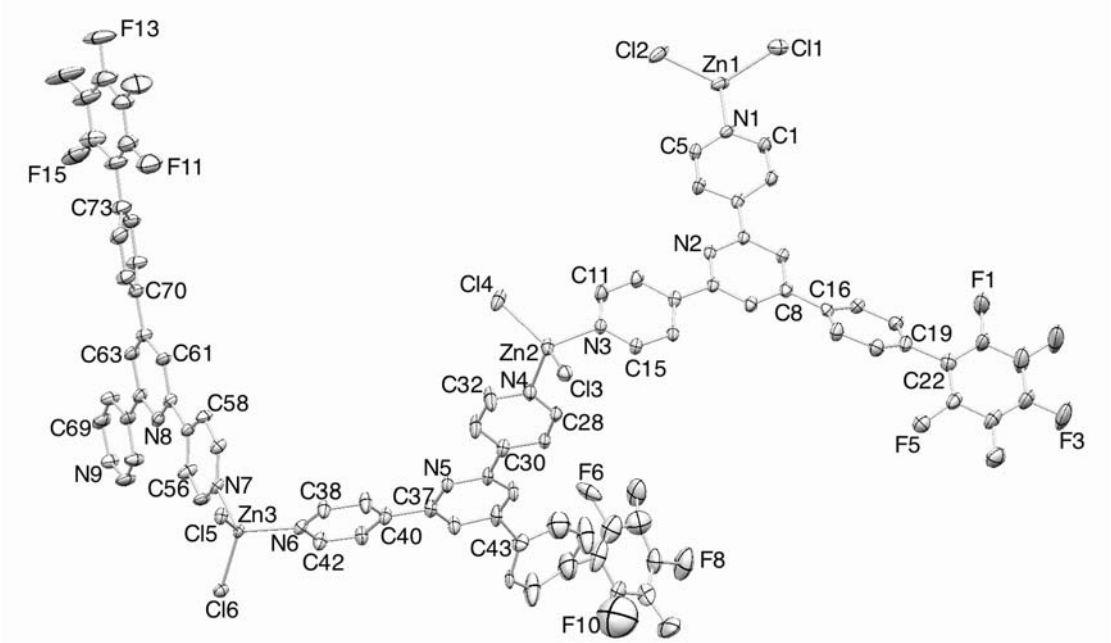

Fig. S5 ORTEP plot with atom labelling for the contents of the asymmetric unit in [{$ZnCl_2$(2)}$_6$]. Ellipsoids plotted at 25% probability level; H atoms and solvent molecules omitted.

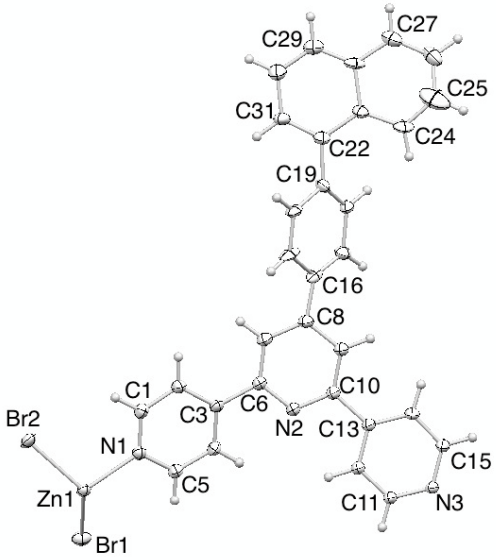

Fig. S6 ORTEP plot with atom labelling for the contents of the asymmetric unit in [{$ZnBr_2$(**3**)}$_6$]·3$CHCl_3$·15H_2O. Ellipsoids plotted at 40% probability level; solvent molecules omitted.

Crystallographic data for [{$ZnCl_2$(**1**/**2**)}$_6$]·2$CHCl_3$·3MeOH·9H_2O (Conformer I)

$C_{167}H_{131}Cl_{18}F_{15}N_{18}O_{12}Zn_6$, M = 3897.04, colourless block, trigonal, space group R–3, a = b = 37.801(3), c = 11.3665(11) Å, U = 14066(2) Å^3, Z = 3, D_c = 1.374 Mg m^{-3}, μ(Cu-Kα) = 3.826 mm^{-1}, T = 123 K. Total 32721 reflections, 5664 unique, R_{int} = 0.0937. Refinement of 3938 reflections (434 parameters) with I >2σ (I)

converged at final $R1$ = 0.0599 ($R1$ all data = 0.0939), $wR2$ = 0.1567 ($wR2$ all data = 0.1769), gof = 1.035. CCDC 956350.