Electronic Supplementary Material (ESI) for Dalton Transactions

Molecular squares, cubes and chains from self-assembly of bis-bidentate bridging ligands with transition metal dications

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Supporting information: details of crystal structures of $[Ni_4(L^{th})_6](BF_4)_8$•*4MeCN and* $[Cu_4(L^{th})_6](BF_4)_8$

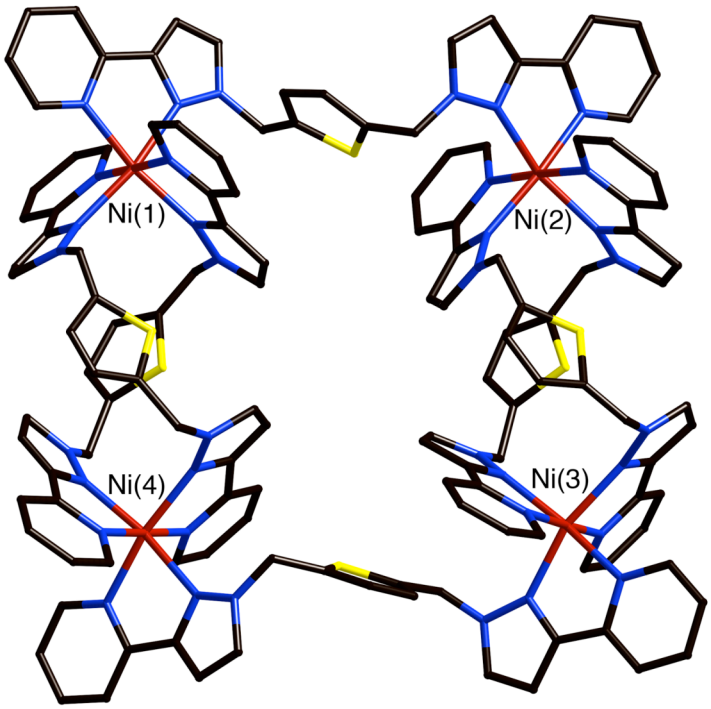

Figure S1. Structure of the complex cation of $[Ni_4(L^{th})_6](BF_4)_8$•4MeCN. The two double helical subunits (Ni1/Ni4 and Ni2/Ni3) have the same chirality but are crystallographically inequivalent. Average bond distances around Ni(1), 2.13Å; Ni(2), 2.10 Å; Ni(3), 2.10 Å; Ni(4), 2.11 Å. Ni(1)•••Ni(4), 9.43 Å; Ni(2)•••Ni(3), 9.08 Å; Ni(1)•••Ni(2), 10.29 Å; Ni(3)•••Ni(4), 10.73 Å.

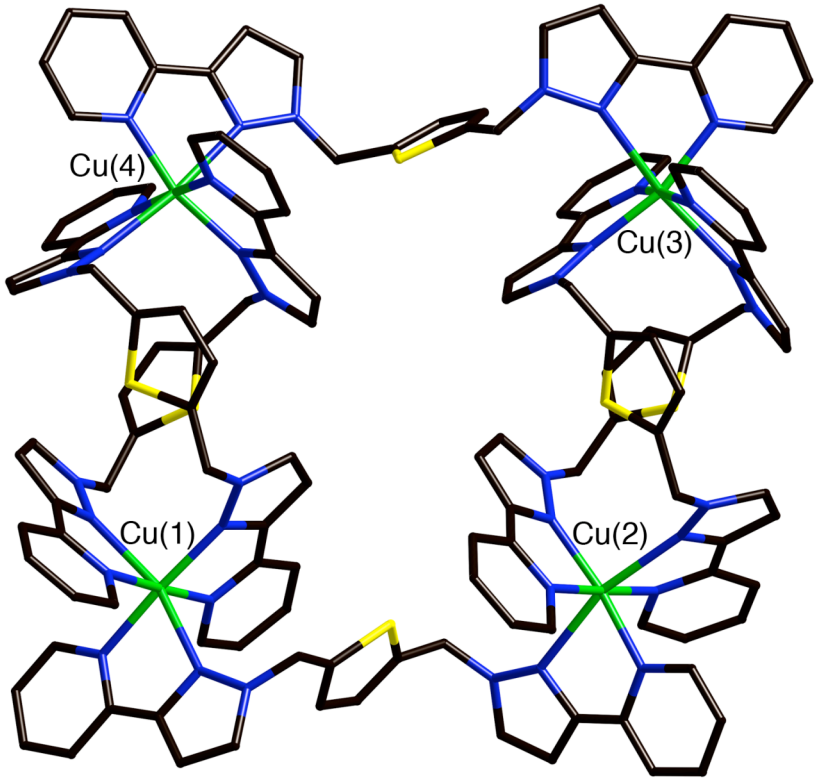

Figure S2. Structure of the complex cation of $[Cu_4(L^{th})_6](BF_4)_8$. The two double helical subunits (Cu1/Cu4 and Cu2/Cu3) have the same chirality but are crystallographically inequivalent. All Cu(II) ions have an axially-elongated coordination geometry with the pyrazole-pyrazole axis being elongated. Average distance of Cu–N bonds in equatorial plane: 2.04 Å. Average distance of long axial Cu–N(pyrazole) bonds: 2.35 Å. Cu(1)•••Cu(4), 9.16 Å; Ni(2)•••Ni(3), 9.25 Å; Cu(1)•••Cu(2), 10.14 Å; Cu(3)•••Cu(4), 11.17 Å.