Summary of data/files

Compound identification

L1 = (±)-2,3,7,8,12,13-Hexa(pyridyl-4-carboxylate)-10,15-dihydro-*5H*-tribenzo[*a,d,g*]cyclononene (trivial name = hexakis(isonicotinoyl)cyclotricatechylene)

Compound 1 = $[Re_3(L1)_2Br_3(CO)_3]\cdot n(CH_3NO_2)\cdot m(H_2O)$

Complex 2a = $[Co_3(H_2O)_6(L1)_2]\cdot 6(NO_3)\cdot n$(dimethylformamide)

Complex 2b = $[Cu_3(H_2O)_6(L1)_2]\cdot 6(NO_3)\cdot n$(dimethylformamide)

Complex 2c = $[Ni_3(H_2O)_6(L1)_2]\cdot 6(NO_3)\cdot n$(dimethylformamide)

Complex 3a = $[Co_3Cl_6(L1)_2]\cdot n$(dimethylformamide)

Complex 3b = $[Co_3Br_6(L1)_2]\cdot n$(dimethylformamide)

Complex 4 = $[Co_3I_{1.5}(H_2O)_{4.5}L1)_2]\cdot 4.5I\cdot m$(dimethylformamide)

Complex 5 = $[Cu_2(L1)(trifluoroacetate)_3$(isonicotinate)$]\cdot n$(dimethylformamide)

Complex 6 = $[Ag_2(L1)(dimethylformamide)_2]\cdot 2BF_4\cdot 2(H_2O)\cdot 6$(dimethylformamide)

NMR.zip

Images (*.PDF) and raw data for Nuclear Magnetic Resonance Data of L1 in dimethylsulfoxide (DMSO) solution

Crystal.zip

Data for single crystal structure determinations

Each folder contains:

- X-Ray data file as name.hkl
- Original data file where SQUEEZE procedure has been used if appropriate
- Final refinement results as name.res
- Crystallographic information file as name.cif
- Structure factor file as name.fcf

Analysis.zip

Additional characterisation data of compounds including:

- Mass spectrum of L1
- Infrared spectroscopy of all compounds (Infrared.pdf)
- Thermogravimetric Analysis Data (TGA data.pdf)
- CHN Elemental analysis results

SEM-EDX.zip

Data and images for energy dispersive X-ray spectroscopy