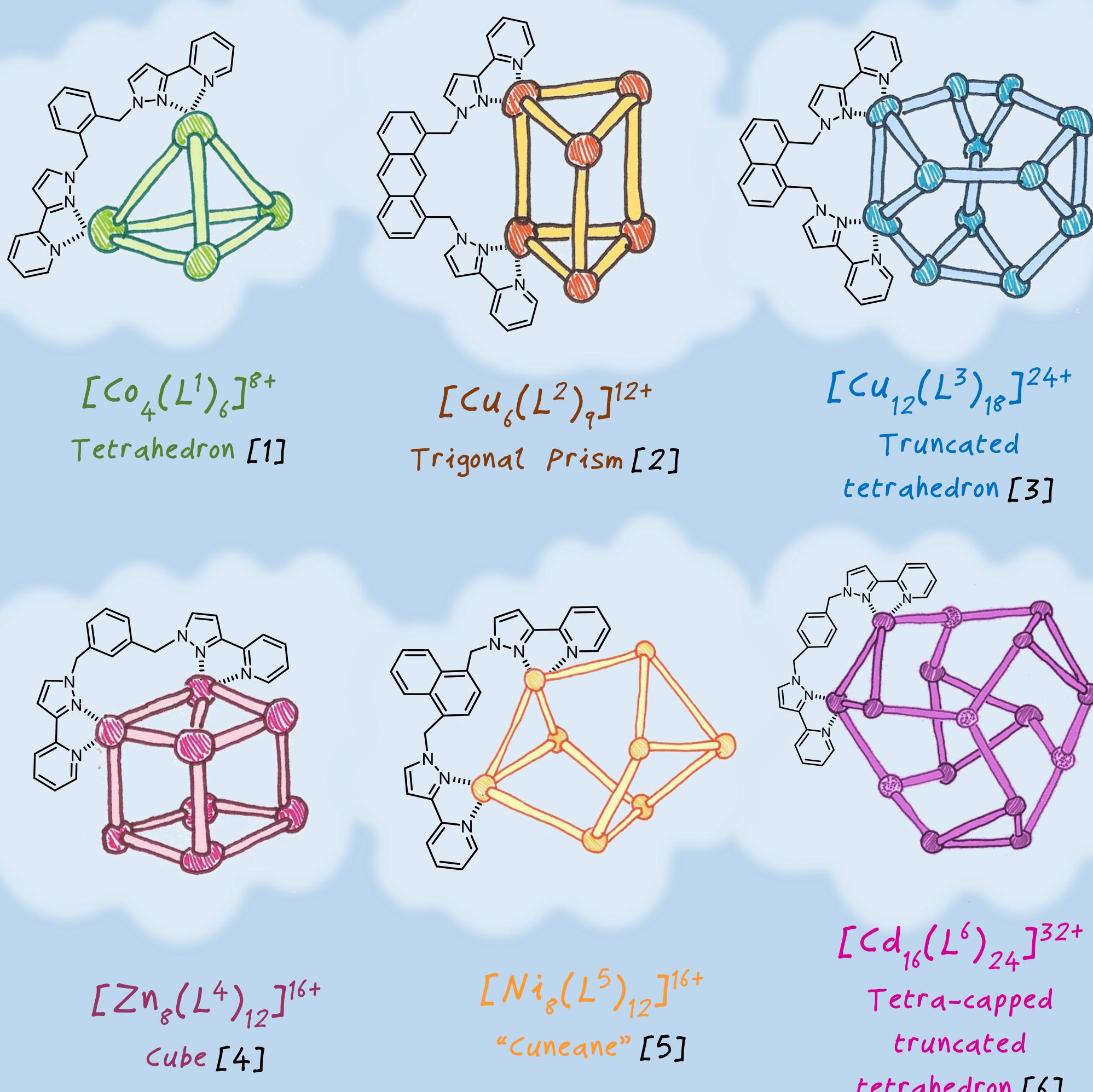


A mixed-ligand coordination cage expands a family of luminescent chemical reactors.

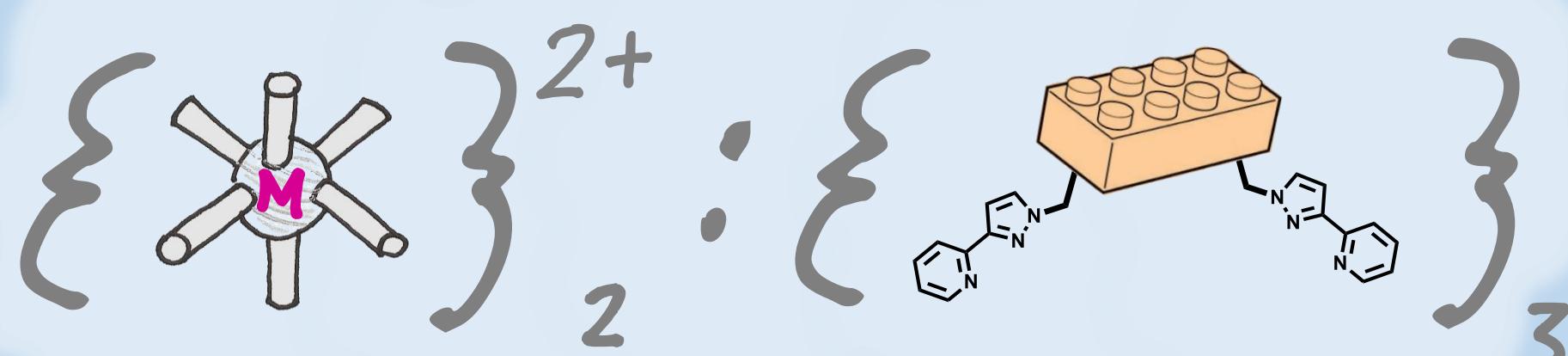


Stephen P. Argent, Fiona Jackson, Justin Chan, Christopher G. P. Taylor, Jon P. Rourke, Michael D. Ward

The story so far... a tale of linkers and polyhedra



A family of bis-bidentate pyrazolyl pyridine ligands $\text{L}^1\text{-}6$ can be combined with variety of M(II) cations to give polyhedral cage complexes. The cages have been variously characterised in the solid state (SCXRD) and solution (NMR & ESI-MS).



The previous cages (left) all have M2:L3 ratios. This is the outcome of combining six-coordinate M^{2+}EN_3 metal cations with tetradentate ligands.

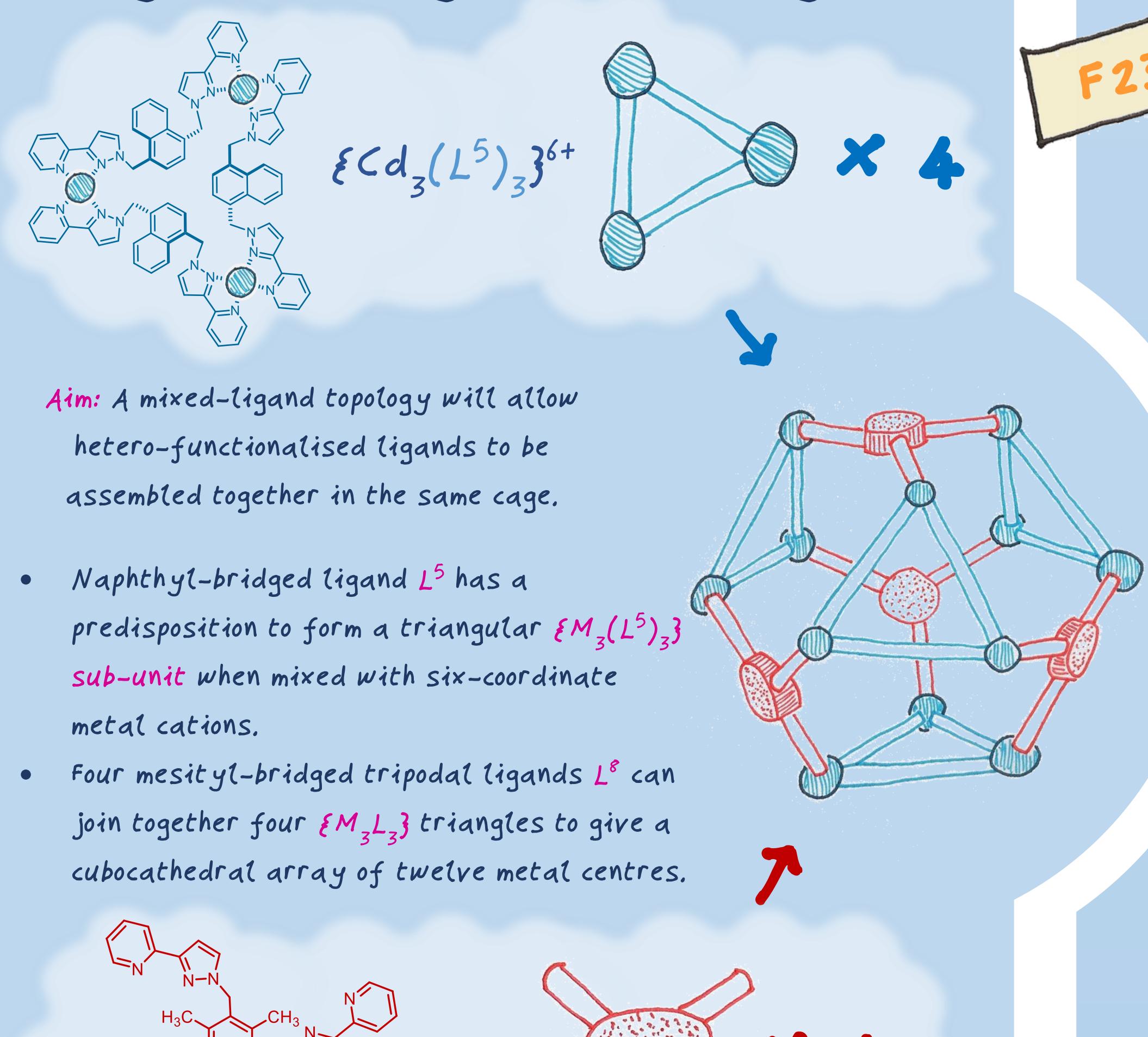
The M2:L3 ratio dictates that the cages must have a three-connected topology i.e. every vertex (metal) connects to three edges (ligands).

Cage topologies prepared so far include Platonic and Archimedean solids, plus a few unusual shapes. [7]

Cage topologies are very hard to predict!

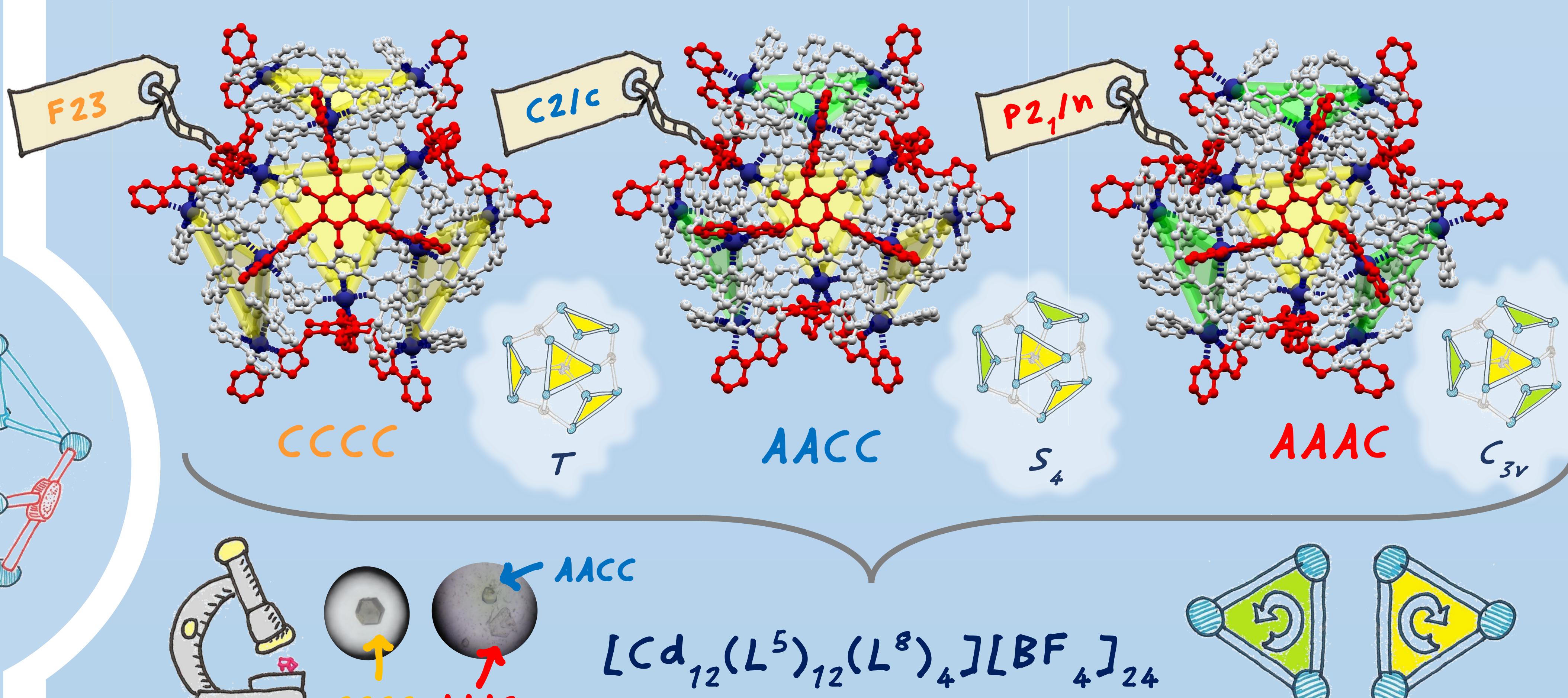


Designing a mixed ligand cage topology



The cuboctahedron is an Archimedean solid (consists of only regular polygons and identical vertices). It is composed of eight triangular and four square faces. The cuboctahedron is four-connected, not three-connected; it can only be constructed using ligands with a mixture of bis- and tris-bidentate ligands. [12]

Cuboctahedron: One Topology - Three Diastereomers



Upon reacting L^5 and L^8 with $\text{Cd}(\text{II})(\text{BF}_4)_2\text{n}(\text{H}_2\text{O})$ a mixture of crystals grow with three distinct morphologies. X-Ray analysis shows that each crystal is a different diastereomer of the $\{\text{Cd}_{12}\}$ cuboctahedron complex.

Analysis of the $\{\text{Cd}_{12}\}$ reaction mixture by ¹H-NMR gives a complex spectrum: all three cage diastereomers are superimposed. Signals for the mesityl-methyl groups (*) of ligand L^8 reveal an almost statistical mixture of the three species.

What next? We will investigate what kind of guests can be accommodated inside the 1,000 Å³ cage cavity.

¹H-NMR (600 MHz, CD_3CN) of $\{\text{Cd}_{12}\}$

