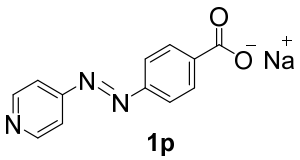
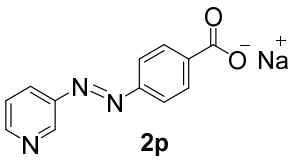
Compound abbreviations and chemical structures:

Precursors:

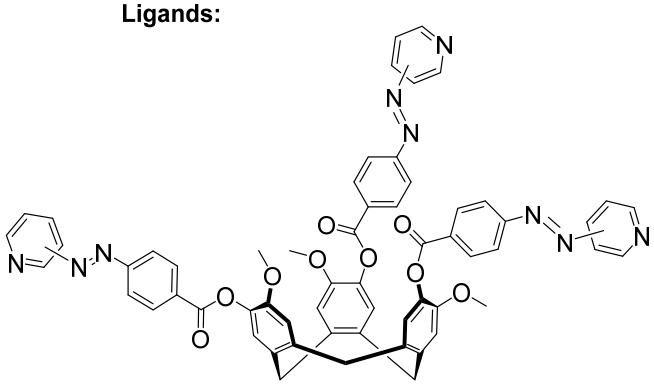


1p

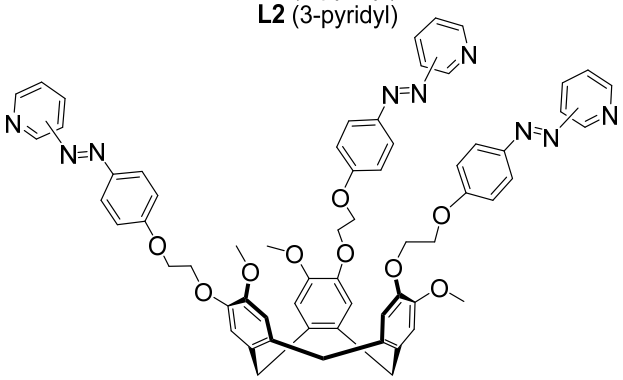


2p

Ligands:

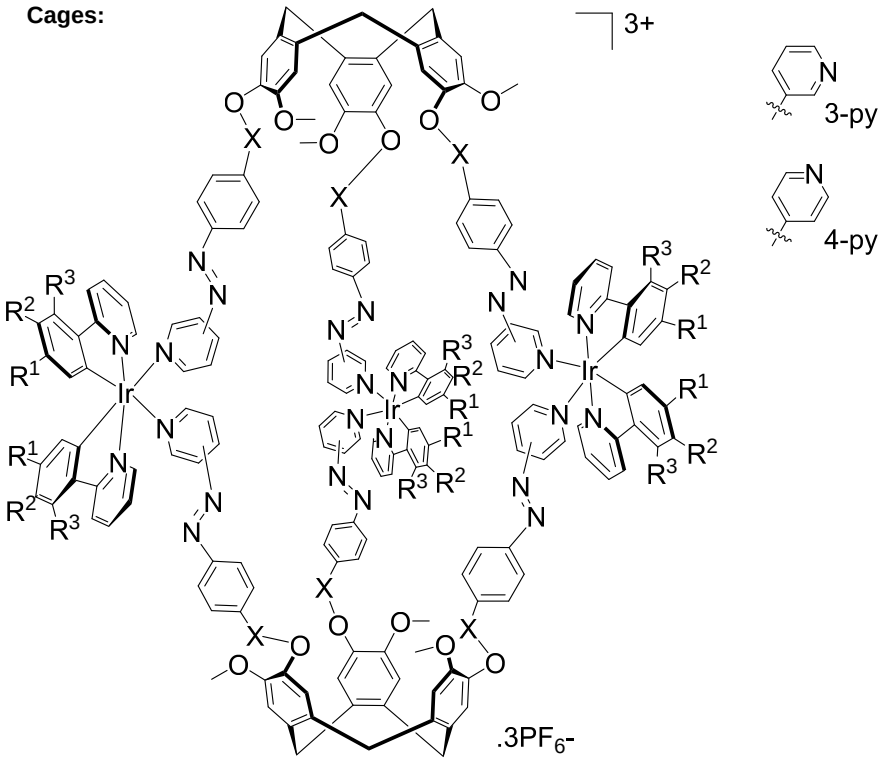


L1 (4-pyridyl)
L2 (3-pyridyl)



L3 (4-pyridyl)
L4 (3-pyridyl)

Cages:



For **L2** with X = C=O, 3-py
R1 = R2 = R3 = H, **C1**
R1 = CH_3; R2 = R3 =H, **C1-Me**
R1 = R2 = R3 = F, **C1-F**

For **L3** with X = (CH_2CH_2O), 4-py
R1 = R2 = R3 = H, **C2**

For **L4** with X = (CH_2CH_2O), 3-py
R1 = R2 = R3 = H, **C3**

Filename	Contents
NMR.zip	Raw data for nuclear magnetic resonance (NMR) experiments used for characterisation, including ^{1}H and ^{13}C experiments recorded. Representative processed spectra as pdf files Spectra were run on a Bruker DPX 300 MHz or Bruker Ascend 400 MHz NMR or Varian Unity Inova 500 MHz (ROESY spectra) or Jeol ECA 600 MHz (DOSY) spectrometer.
Other characterisation.zip	Infrared spectra, mass spectra, UV-visible data and microanalysis results for characterisation of ligands, precursors and cages
Xray.zip	CIF (crystallographic information files) for single crystal X-ray structures with separate or embedded structure factor (.fcf) information.

Photoisomerisation.zip	UV-visible data, mass spectrometry, NMR spectroscopy to support photoswitching experiments of ligands and cages
Photophysics.zip	Luminescence emission data for cages with lifetime studies