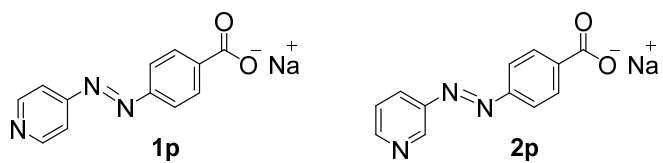
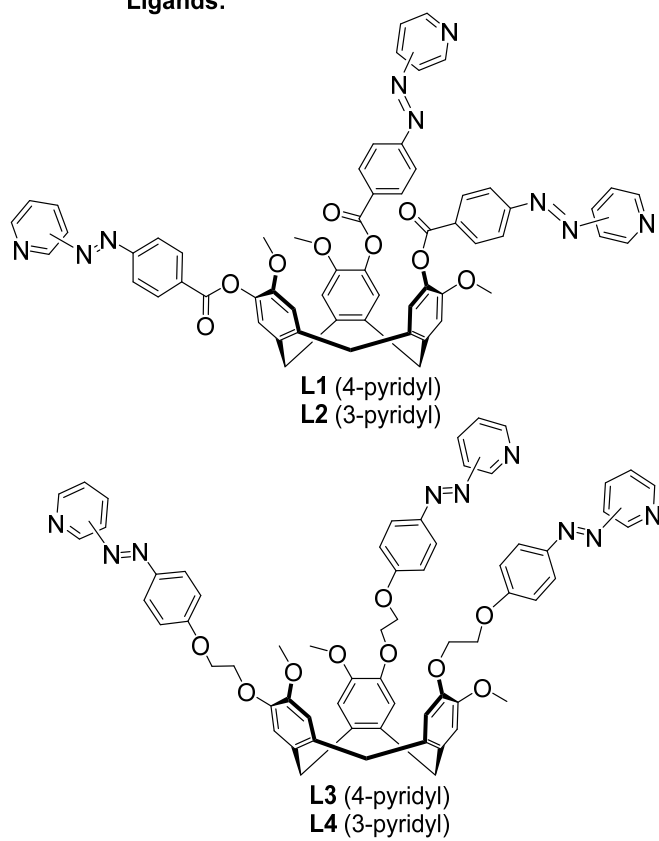


Compound abbreviations and chemical structures:

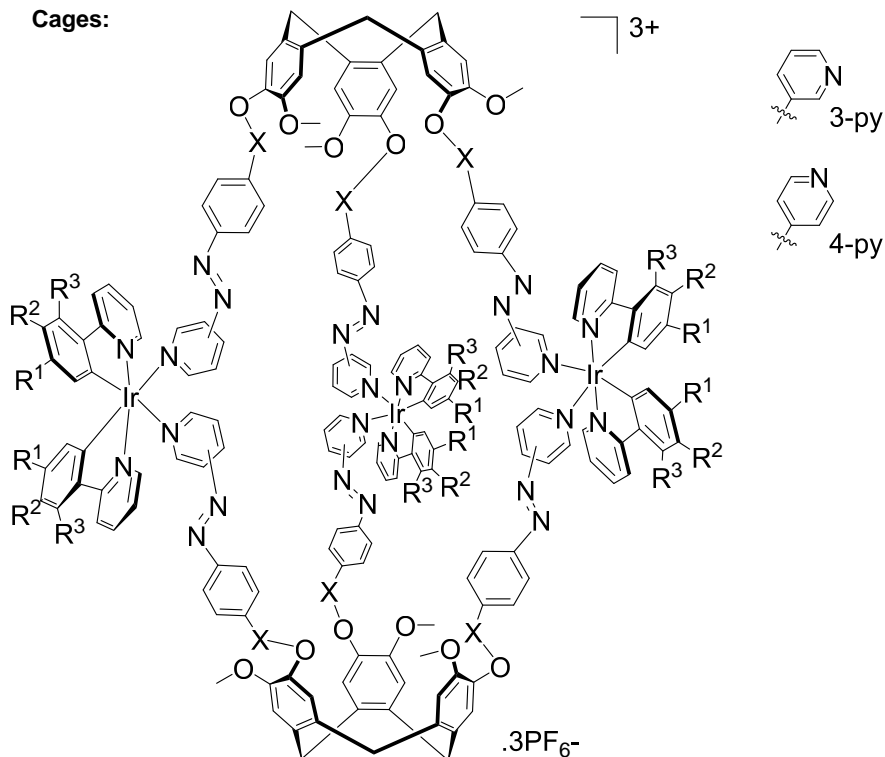
Precursors:



Ligands:



Cages:



For **L2** with X = C=O, 3-py
 R1 = R2 = R3 = H, **C1**
 R1 = CH₃; R2 = R3 = H, **C1-Me**
 R1 = R2 = R3 = F, **C1-F**

For **L3** with X = (CH₂CH₂O), 4-py
 R1 = R2 = R3 = H, **C2**

For **L4** with X = (CH₂CH₂O), 3-py
 R1 = R2 = R3 = H, **C3**

Filename	Contents
NMR.zip	<p>Raw data for nuclear magnetic resonance (NMR) experiments used for characterisation, including ¹H and ¹³C experiments recorded.</p> <p>Representative processed spectra as pdf files</p> <p>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.</p>
Other characterisation.zip	<p>Infrared spectra, mass spectra, UV-visible data and microanalysis results for characterisation of ligands, precursors and cages</p>
Xray.zip	<p>CIF (crystallographic information files) for single crystal X-ray structures with separate or embedded structure factor (.fcf) information.</p>

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