

Poster Presentation

MS67.P11

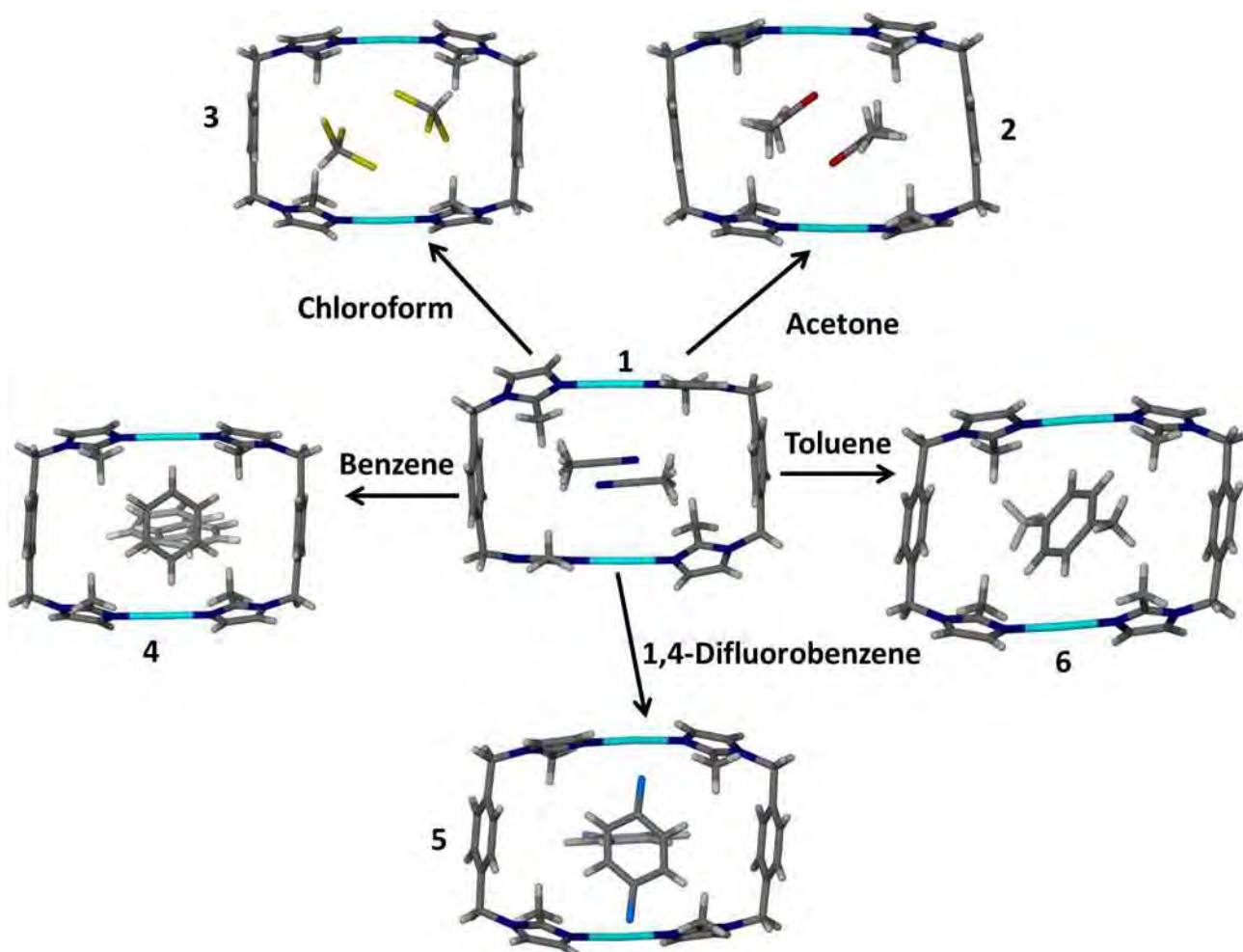
Single-crystal guest exchange and phase transformations in a porous metallocycle

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One of the target architectures for porous crystals investigated by our group is the “doughnut-shaped” metallocycle. The “doughnut” shape of the metallocycles prevents them from packing efficiently and results in the formation of crevices, cavities or channels in the packing arrangement. Naturally, owing to close-packing requirements the occurrence of empty space in the crystal structure is energetically unfavourable and therefore the available “space” is usually occupied by solvent molecules. Ideally, the porous phase can be obtained by removing the solvent molecules from the channels without disrupting the host framework. In this regard we have conducted a further investigation of the porous metallocycle previously reported by Barbour et al.[1] Single crystals of a previously reported porous metallocycle $[\text{Ag}_2\text{L}_2](\text{BF}_4)_2 \cdot 2\text{CH}_3\text{CN}$ (1) were grown from acetonitrile and immersed in different organic solvents. The crystals thus treated were subjected to single-crystal X-ray diffraction analysis, which revealed that the acetonitrile guest molecules had been replaced by the solvent that the compound was exposed to, yielding five different solvates: $[\text{Ag}_2\text{L}_2](\text{BF}_4)_2 \cdot 2(\text{CH}_3)_2\text{CO}$ (2), $[\text{Ag}_2\text{L}_2](\text{BF}_4)_2 \cdot 2\text{CHCl}_3$ (3), $[\text{Ag}_2\text{L}_2](\text{BF}_4)_2 \cdot \text{C}_6\text{H}_6$ (4), $[\text{Ag}_2\text{L}_2](\text{BF}_4)_2 \cdot \text{C}_6\text{H}_4\text{F}_2$ (5), $[\text{Ag}_2\text{L}_2](\text{BF}_4)_2 \cdot \text{C}_7\text{H}_8$ (6). Thermogravimetric analysis supports these findings.

[1] L. Dobrzańska, G. O. Lloyd, H. G. Raubenheimer, et al., *J. Am. Chem. Soc.*, 2005, 127, 13134.



Keywords: Single-crystal, guest exchange, phase transformations