

## MS29 Crystal engineering: structural flexibility, phase transitions and non-standard manipulation of synthons

MS29-03

Carboxylate metallogels and coordination networks: the role of non-covalent interactions

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### Abstract

Supramolecular interactions form the basis for a range of functional materials. The study of non-covalent interactions (NCIs), and the supramolecular synthons they form, has reached a mature phase. Thus crystal engineering of functional solid materials has grown into a vibrant and exciting field. Related to crystal engineering, through the use of the same NCIs and supramolecular synthons is the field of soft materials. Together, these areas allow researchers to prepare a range of stimuli-responsive materials,<sup>1-3</sup> such as supramolecular gels, metal-organic networks (MOFs), covalent organic frameworks (COFs), and other porous coordination networks. These materials are then of use in catalysis, drug delivery, gas storage, separation and sensing.

As part of a study investigating the factors affecting the formation of supramolecular gels,<sup>4</sup> we considered a range of di- and tri-carboxylic acid linkers, including 2,6-pyridinedicarboxylic acid (26pca), 3,5-pyridinedicarboxylic acid (35pca), and benzene-1,3,5-tricarboxylic acid (btc). The key factors required in linkers are the capacity to form porous networks; having three groups capable of forming NCIs is favourable, eg. btc and 35pca. 26pca was not useful in producing gels, as it lacks the 3<sup>rd</sup> anchoring point. However, three crystalline compounds of this linker with Fe(III) provided a case study<sup>5</sup> in the influence of reaction time and temperature on the nature of the NCIs and hence the complexity and stability of the structures obtained (Figure 1). We found that btc could be used to form both gels and single crystals, through similar NCIs. A survey of related structures in the CSD<sup>6</sup> found there are four common topological motifs (Figure 2), which cannot be predicted from either the composition or space group of the compound.<sup>7</sup>

### References

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Fig 1. Structures of 26pca with Fe(III)

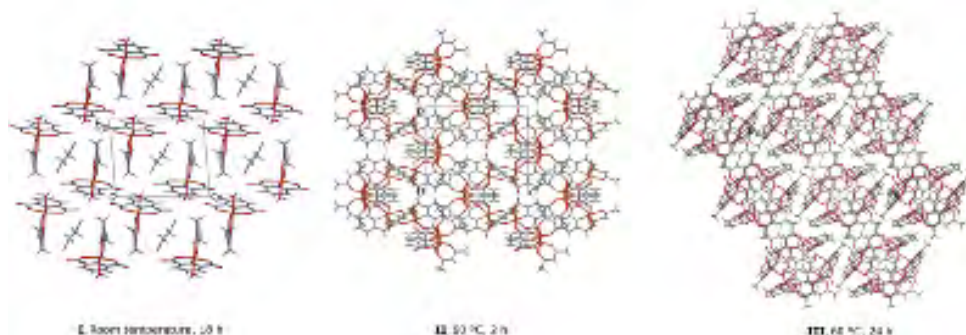


Fig 2 Motifs observed in btc coordination polymers

