Electronic Supplementary Information (ESI) for CrystEngComm

Conformation variation of tris(2-carboxyethyl)isocyanuric acid induced by cocrystallized N-heterocyclic organic molecules

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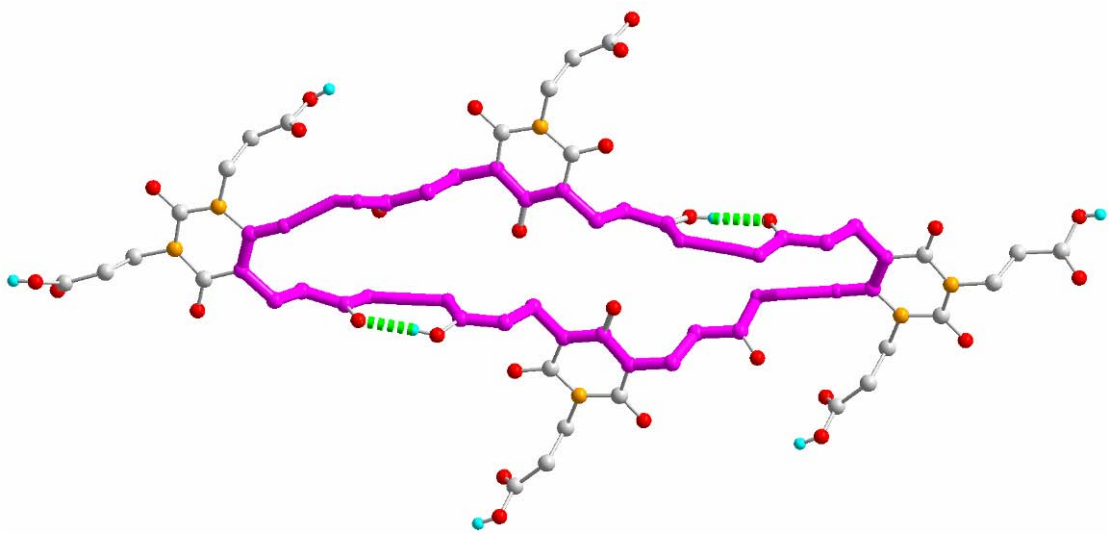
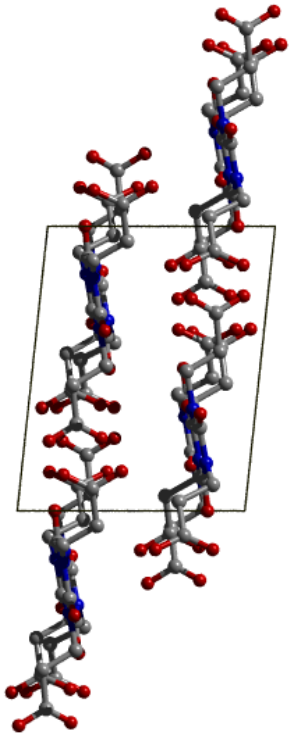
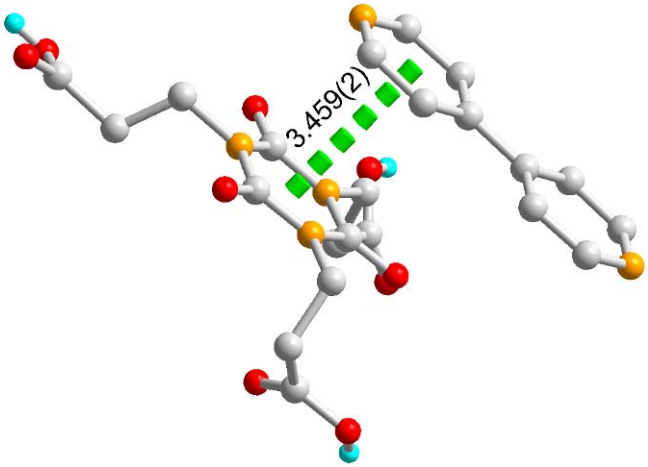
(1) Figure S1. 40-membered supramolecular macrocycle in **1.**



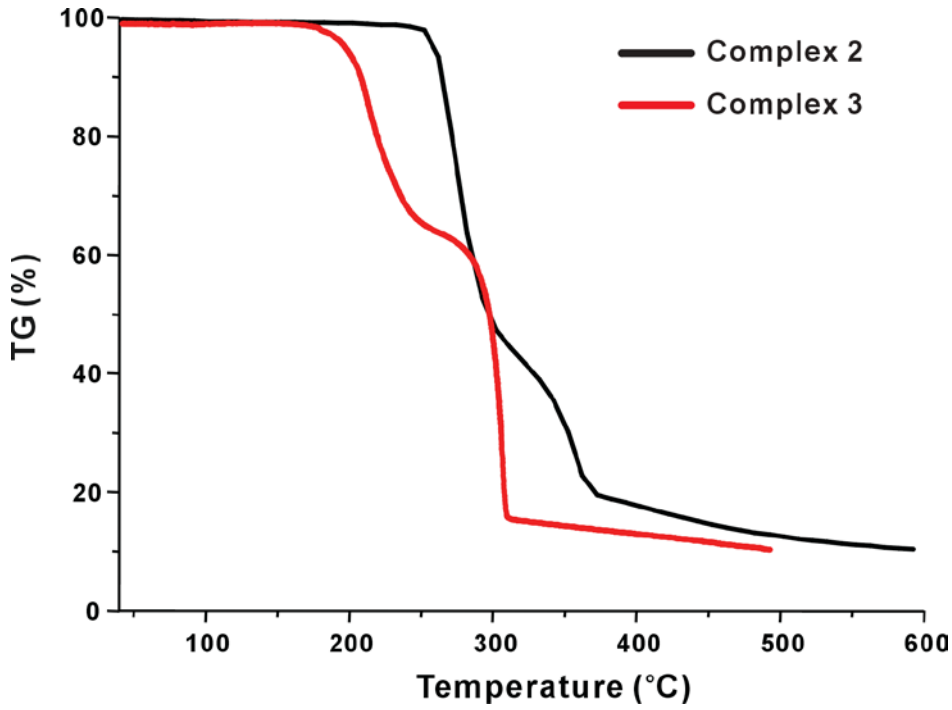
(2) Figure S2. Packing of the 2D sheets in complex **1** along *b* axis in one unit cell.



(3) Figure S3. The face-to-face π···π □interaction in complex **3.**



(4) Figure S4 TGA for complexes **2** and **3.**



(5) Table S1 The CSD search of the reported conformations of H_3tci.

Refcode	Conformation	Reference
WAJFEU	*cis*^{gauche}-*cis*^{gauche}-*cis*^{gauche} and *cis*^{anti}-*cis*^{anti}-*trans*^{anti}	Inorg. Chem., 2010, 49, 769
RULNES	*cis*^{anti}-*cis*^{anti}-*trans*^{anti}	Adv. Inorg. Biochem., 2009, 4, 870
RULNIW	*cis*^{gauche}-*cis*^{gauche}-*cis*^{gauche} and *cis*^{anti}-*cis*^{anti}-*trans*^{anti}	Adv. Inorg. Biochem., 2009, 4, 870
RULNOC	*cis*^{anti}-*cis*^{gauche}-*trans*^{gauche}	Adv. Inorg. Biochem., 2009, 4, 870
TOHYOF	*cis*^{anti}-*cis*^{anti}-*trans*^{anti}	CrystEngComm, 2008, 10, 1739
TOHYUL	*cis*^{anti}-*cis*^{anti}-*trans*^{anti} and *cis*^{anti}-*cis*^{anti}-*trans*^{anti}	CrystEngComm, 2008, 10, 1739
TOHZAS	*cis*^{anti}-*cis*^{anti}-*trans*^{anti}	CrystEngComm, 2008, 10, 1739
XOLROG	*cis*^{anti}-*cis*^{anti}-*cis*^{anti}	Angew. Chem., Int. Ed. 2008, 47, 8843
XOLRUM	*cis*^{anti}-*cis*^{anti}-*cis*^{gauche} and *cis*^{anti}-*cis*^{anti}-*cis*^{gauche}	Angew. Chem., Int. Ed. 2008, 47, 8843