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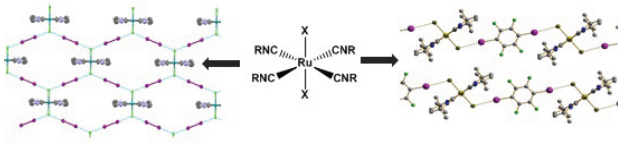

Figure 1.

Keywords: Halogen Bonding, Substitution Reactions

MS32-O4 Engineering ternary cocrystals by orthogonal hydrogen and halogen bonds

Filip Topić[1], Kari Rissanen[1]

1. University of Jyvaskyla, Department of Chemistry, Nanoscience Center, P.O. Box 35, FI-40014 University of Jyvaskyla, Finland

email: filip.f.topic@jyu.fi

In the still maturing field of halogen bonding, we have been especially interested in discovering new halogen bonding motifs [1,2] and applying them in crystal engineering [3].

The particular robustness of C–I···S halogen bond with thioureas has recently been highlighted, persisting even in solution [4], In addition to that, the orthogonality of such interaction to hydrogen bonds has also been demonstrated [5], offering the possibility of constructing complex systems where the two can operate independently.

Also knowing that the crown ethers reliably cocrystallize with thioureas [6,7], this prompted us to combine thioureas with crown ethers and various (aromatic and non-aromatic) perfluorinated halogen bond donors, resulting in a large number of ternary cocrystals with high supramolecular yield. Besides the success of the strategy and the aesthetically appealing structures, these systems present other intriguing aspects, such as differing behavior of bromine- and iodine-based donors, tunable metrics and, finally, the possibility of constructing porous materials.

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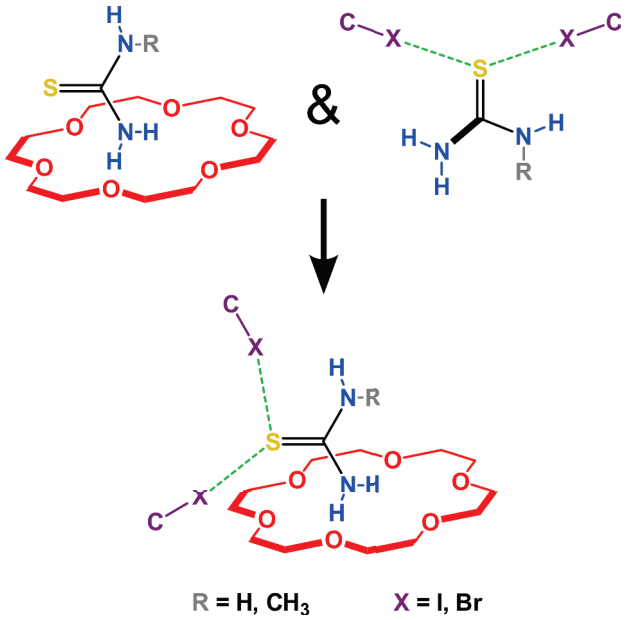

Figure 1. Hydrogen and halogen bonded motifs are combined in the studied ternary cocrystals.

Keywords: crystal engineering, ternary co-crystals, hydrogen bond, halogen bond, orthogonality

MS32-O5 Halogen bonding in host-guest compounds: Structures and kinetics of enclathration and desolvation

Francoise Mystere Amombo Noa[1], Susan Ann Bourne[1], Luigi Renzo Nassimbeni[1]

1. Centre for Supramolecular Chemistry, Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa.

email: noa.mystere@gmail.com

The host compounds tetrakis-(4-bromophenyl) ethylene and its iodo-analogue form inclusion compounds with a series of chloro- and iodo-methanes. Their structures have been elucidated and their non-bonded halogen···halogen contacts analysed and classified. Their kinetics of desolvation have been studied and the concomitant activation energies established. The velocity of the enclathration for the solid-methyl iodide vapour reactions and associate rate law have been established. Figure 1 shows halogen· ··halogen interactions between the host compound tetrakis-(4-bromophenyl) ethylene and the guest diiodomethane.

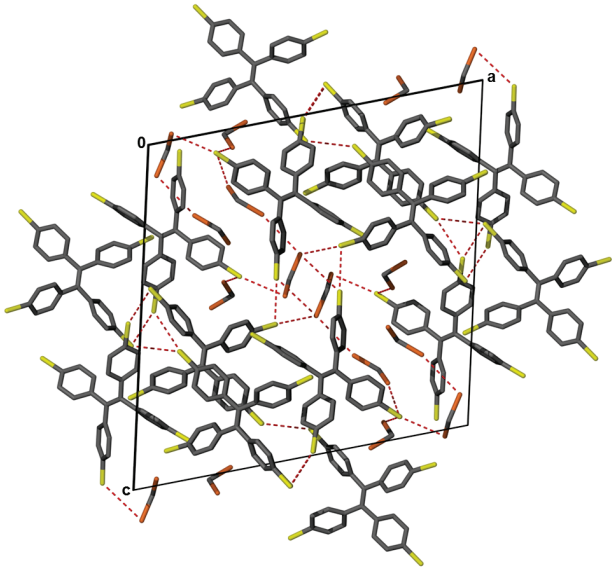

Figure 1. Packing diagram of tris diiodomethane bis tetrakis-(4-bromophenyl) ethylene along [010] showing halogen···halogen interactions.

Keywords: Halogen-halogen interactions, halogen bonding