Structural features of the formation of Hydrogen bonded Organic Frameworks

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MOFs, COFs and HOFs as highly ordered porous architectures attract wide interest owing to their broad potential of application in heterogeneous catalysis, storage, sensing, drug delivery, separation, etc.

Research of organic frameworks assembled by supramolecular interactions without metal or covalent bonds taking part in the framework construction has come in the focus of interest the most recently. A well-orchestrated interplay of supramolecular interactions, molecular inflexibility and spatial effects characterize the non-covalently bonded organic frameworks. All mentioned aspects affect the molecular and crystal symmetries. We reported recently the preparations and structures of ionic hydrogen-bonded organic frameworks, their polymorphic and solvatomorphic forms were described [1]. Further attempts were made to prepare hydrogen bonded organic frameworks, either ionic or neutral. Our systematic study inspired by the Maruoka type chiral phase-transfer catalysts resulted in some new series of solvatomorphic hydrogen bonded organic framework materials. We will present (Fig. 1), that the most important aspects in the HOF formation include (1) the intramolecular interactions which are responsible for the inflexibility of the molecule, (2) the intermolecular interactions which are responsible for framework construction, (3) the terminal spacer groups for void formation, (4) the molecular symmetries which prove to be important in the tightening of the molecule, and (5) all the afore mentioned features affect the crystal symmetry which may coincide with the molecular symmetry.

The presented work contributes to the understanding of hydrogen bonded organic framework formation. It supports the still challenging design and preparation of framework structures with high porosity.

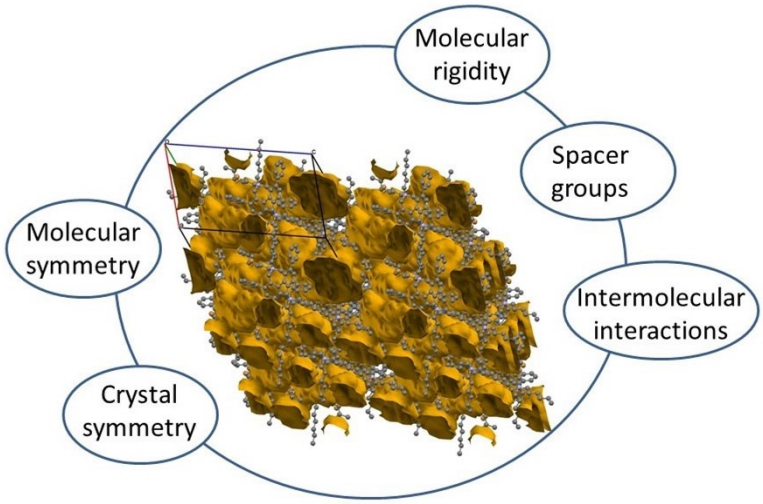

Figure 1. The most important aspects in the HOF formation.

[1] Horváth D. V., Holczbauer T., Bereczki L., Palkó R., May N. V., Soós T., Bombicz P. (2018) *CrystEngComm*, **20**, 1779-1782.

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