

*Supramolecular synthetic protocols for targeting specific topologies of metal-containing solids*

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A prerequisite for practical crystal engineering, with a focus on delivering new materials with targeted properties, is certainly a set of guidelines on how supramolecular building units are likely to assemble in the solid state. While the organic solid-state has already derived numerous productive strategies for non-covalent synthesis by identifying synthons that provide effective avenues for supramolecular synthesis, [1] reliable synthetic strategies that employ a combination of coordinate-covalent bonds and relatively weak and readily reversible hydrogen and/or halogen bonds have not received anywhere near the same attention.

With the idea in mind to develop robust synthetic strategies for targeting specific topologies of metal-containing crystalline solids, we have focused on several functionalities that have already been well established to form robust and reliable supramolecular synthons in purely organic systems. In metal-organic systems, on the other hand, being exposed to a number of additional good hydrogen/halogen bond acceptors, the same functionalities are often in a position to opt for new competitors instead of forming the synthons observed in analogous organic systems. Here, we have carried out a systematic structural examination of a series of metal(II) complexes with various pyridine-type- and charge-balancing ligands, and complemented the experimental efforts by an in-depth theoretical analysis of molecular electrostatic potential surfaces to rationalize the observed structural features. Here we will demonstrate how to derive supramolecular synthetic protocols to target the desired supramolecular outcome in much the same way as organic synthesis is systematically altered and refined in response to product yields.[2] Also, we will present on several examples what supramolecular reaction conditions need to be met to be in a position to simply transfer specific supramolecular synthons from organic to metal-organic systems.[3]

Acknowledgment: This work has been fully supported by Croatian Science Foundation under the project UIP-11-2013-1809.

[1] Aakeröy, C.B.; Wijethunga, T.K.; Desper, J. & Đaković, M. (2016) *Cryst. Growth Des.* 16, 2662–2670.

[2] Kukovec, B.-M.; Malik, M.; Kodrin, I.; Aakeröy, C.B. & Đaković, M. (2016) *Cryst. Growth Des.* 16, 7308-7317.

[3] Đaković, M.; Soldin, Ž.; Kukovec, B.-M.; Kodrin, I.; Aakeröy, C.B.; Baus, N. & Rinkovec, T., submitted

**Keywords:** [supramolecular synthons](#), [molecular electrostatic potential](#), [supramolecular synthesis](#)