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predavaonica III. krila IRB-a  
i putem interneta, 11:00 sati

## SUPRAMOLECULAR CRYSTALLOGRAPHY

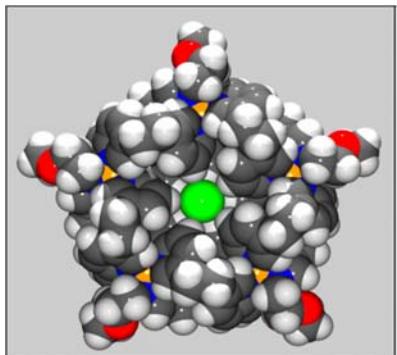


Figure 1. The X-ray structure of the pentafoil knot.

An exciting research challenge in supramolecular chemistry is to design, synthesize, and characterize nano-sized architectures with applications in biology, chemistry, and materials science [1]. Predicting and designing non-covalently bound supramolecular complexes and assemblies is difficult because of the weakness of the interactions involved, thus the resulting superstructure is often a compromise between the geometrical constraints of the building blocks and the competing weak intermolecular interactions [2]. Our research interest has been focused on the studies of weak non-covalent intermolecular, viz. supramolecular interactions as the driving force in self-assembly and molecular recognition, especially in the solid state by single crystal X-ray diffraction. The lecture will highlight some of our recent studies on halogen bonded systems, anion... $\pi$  interactions and metal ion coordination in molecular self-assembly and molecular recognition in various systems such as rotaxanes, knots (Figure 1), M4L6 tetrahedra, M8L6 cube and spheres [3].

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- [2] (a) Desiraju, G.R., *Nature* **2001**, 397; (b) Steiner, T., *Angew. Chem. Int. Ed.* **2002**, 41.
- [3] (a) Ward, J. S.; Fiorini, G.; Frontera, A.; Rissanen, K., *Chem. Commun.* **2020**, 8428; (b) S. Yu, J. S. Ward, K.-N. Truong, K. Rissanen, *Angew. Chem. Int. Ed.* **2021**, 20739; (c) R. Puttreddy, J. M. Rautiainen, S. Yu, K. Rissanen, *Angew. Chem. Int. Ed.* **2023**, e2023073; (d) Inokuma, Y.; Yoshioka, S.; Ariyoshi, J.; Arai, T. Matsunaga, S.; Takada, K.; Rissanen, K.; Fujita, M., *Nature* **2013**, 461; (e) Bunzen, J.; Iwasa, J.; Bonakdarzadeh, P.; Numase, E.; Rissanen, K.; Sato, S.; Fujita, M., *Angew. Chem.* **2012**, 3161; (f) Ayme, J.-F.; Beves, J. E.; Leigh, D. A.; McBurney, R. T.; Rissanen, K.; Schultz, D., *Nat. Chem.* **2012**, 15; (g) Meng, W.; Breiner, B.; Rissanen, K.; Thoburn, J. D.; Clegg, J. K.; Nitschke, J. R. *Angew. Chem.* **2011**, 3479; (h) Mal, P.; Breiner, B.; Rissanen, K.; Nitschke, J. R., *Science* **2009**, 1697.