## MS46 Computational tools for theoretical chemistry in crystallography

Chairs: Martin Lutz, Martyn Winn

### MS46-P1 Topological analysis of self-catenated motifs in coordination networks

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In the last decade, the phenomenon of self-catenation became widespread in structures of coordination compounds[1]. Self-catenation is the entanglement of circular fragments of the same atomic net. Despite the prevalence of the phenomenon among coordination polymers, neither total number of self-catenated structures, nor their topological characteristics (topological type, methods of entanglements of rings) are known yet. The modern crystallochemical approaches in the analysis of such structures are construction of Hopf ring net[2] as well as splitting of the atomic net on the individual entangled motifs[3]. Both approaches are automated and implemented in the program package ToposPro (http://topospro.com)[4]. Thus, our work was devoted to the topological analysis of self-catenated motifs in framework coordination polymers by the ToposPro tools.

At the first step, we have extracted the crystal structural information from the Cambridge Structural Database (version 5.35)[5] for more than 15,000 structures of 3-periodic coordination polymers. Analysis of the structures without topologically dense structural groups (atomic clusters), more than 250 self-catenated frameworks were found. For them we have analyzed all possible ways for splitting into subnets (the most typical of which are – dia, srs, hcb, sql, 4T13) and the topology of entanglements by constructing Hopf's ring net. Using the results we have found general crystallochemical principles of the self-catenation realization .

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