

Structure and properties of hybrid metal-organic nanocages: a combination of Molecular Modelling and X-Ray diffraction techniques

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In this contribution, some of the features of poly-[n]-catenanes composed of interlocked M₁₂L₈ icosahedral nanometric cages are presented. The study includes a combination of X-ray diffraction experiments and Molecular Modelling simulations [1-3]. The materials under investigation is obtained by the usage of TPB (exotridentate trispyridyl benzene) ligand and ZnX₂ (with X=Cl, Br, I): with appropriate templating solvent molecules metal-organic interlocked nanocages microcrystalline materials are formed. X-ray diffraction data allowed to solve the structure and to detect guest molecules exchange processes together with crystal to crystal phase transition phenomena. The processes of crystallization, absorption/release of guests and crystal to crystal transitions are driven by intramolecular and intermolecular interactions. QM calculations specific for the solid phases [4-6] were used to rationalize the observed features permitting to highlight the underlying key factors by a simple hierarchical mechanism of "closed-open" dynamic channels. The capability of specific molecular absorption/release together with the labile nature of the Zn-N coordination bonds allow for the recyclability of TPB ligand and make these materials potential good candidates in green chemistry processes and in molecular sensing and in drug delivery (for example paracetamol) applications.

References

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