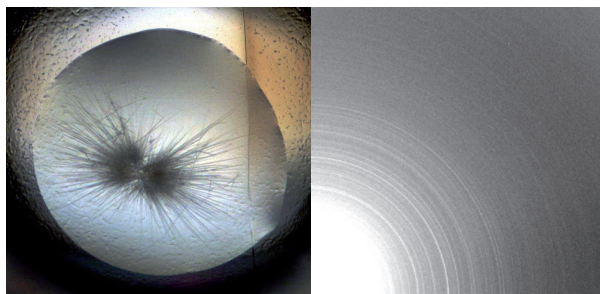


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Measuring on a single urchin like crystal at room temperature used to be unrealistic due to the absence of a reliable available setup. In air, the samples were dehydrated, and measuring a small amount of protein powder sample in a capillary is also difficult. Also, for fragile samples, the centrifuging of microcrystals in a capillary may be fatal for diffraction. We have seen that the design of the humidity control device available at the ESRF allowed us to collect high quality powder diffraction pattern on a PX beamline on a single urchin like crystal. The possibility to preserve small protein powder samples at room temperature without losing diffraction properties is a new step for protein powder diffraction. This allows several possibilities, first, to screen very easily and routinely crystalline precipitates in order to determine their diffraction quality, on any PX beamline; second, to get reliable intensities at low to medium resolution, suitable to solve a structure by molecular replacement; third, to build and refine a preliminary model using these extracted intensities or via a Rietveld refinement.

Data acquisition and preliminary analysis on the non structural protein 3 macro domain of the Mayaro virus will be presented, following previous studies[1] done on a larger amount of sample.



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Solid state reactivity and solvent mobility in crystals of a cubane polymer

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Solids that accommodate small molecules in structural voids are of interest for applications as diverse as catalysis or gas storage and purification. Most systems studied to date in this area are 2- and 3-D polymers with frameworks that maintain open voids. In contrast, 1-D polymers give structures without rigidity in three dimensions, so removal of small molecules that might be present leads to the collapse of the crystal structure. Moreover, solids formed by 1-D polymers usually have a lesser amount of void space to house solvent and other small molecules.

To understand the storage of small molecules in solids, it is necessary to characterize the geometries of the pores or voids involved, and also their chemical nature. The study of solid-state reactions provides insight into both the chemical and physical natures of the substances and processes involved. [2]

Quadruply deprotonated citrate forms transition metal complexes with a topologically cubic M_4O_4 core and 12 peripheral oxygen atoms that can bind transition metals or form non-covalent interactions with interstitial small molecules. The cubane units are structural building blocks for polymers of varying dimensionality; their hydrophilic periphery confers exceptional qualities on the solids, including structural variability, water solubility and solid-state chemical reactivity. [4,5]

We have previously reported an unprecedented solid-state crosslinking in which a 1-D polymer of cobalt citrate cubanes fuses under mild conditions to produce a 2D polymer. [5] This quasi-topotactic process demonstrates the structural flexibility and solid-state reactivity typical of these compounds and suggests the possibility of studying the reaction mechanisms of the solid state transformations.

We present here a new family of non-porous 1-D and 2-D manganese citrate cubane polymers whose flexible structural natures permit the reversible desorption of water in SCSC transformations at room temperature. Both species have mobile interstitial water molecules. There are no clearly defined voids or channels for water mobility, so the structural framework must yield in order for water egress and reuptake to take place. In addition, if the dehydrated derivative of the 1-D polymer is exposed to a methanol atmosphere, one molecule of methanol substitutes an aqua ligand on a non-cubane manganese(II) unit present in the structure, through a possible associative mechanism. This reversible transformation preserves the crystallinity of the polymer. There is evidence that one more molecule of methanol enters the polymer through a physisorption process.

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Flexibility found in silica-like metal-organic frameworks

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Throughout the last decade, the study of metal-organic frameworks (MOFs) has remained one of the most topical fields in solid-state chemistry, due to the extensive and unique range of structural and functional properties they exhibit [1].

In recent years, studies on MOFs have revealed unusual mechanical properties, such as negative thermal expansion in MOF-5 [2], and amorphisation of zeolitic imidazolate frameworks at high temperature [3].

This poster will be focused on mechanical properties of some MOFs whose structures resemble those of silicate frameworks. For example, cadmium and mercury imidazolates (with a topological resemblance to α -cristobalite), have shown unusual thermal expansion