Poster Presentation

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Fructose calcium chloride MOFs for NLO applications

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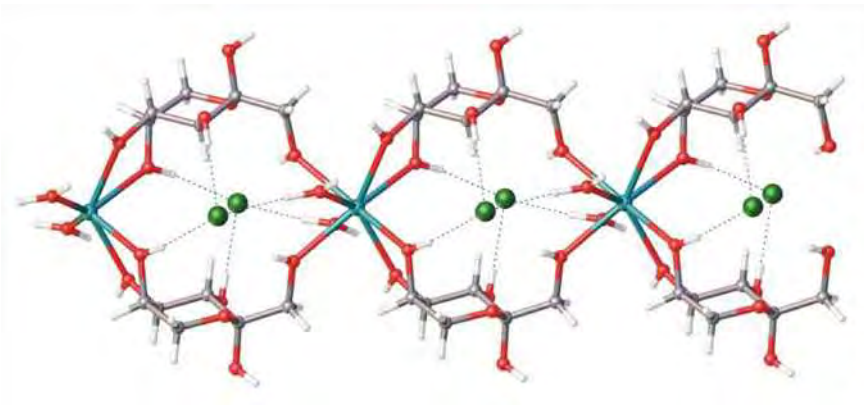
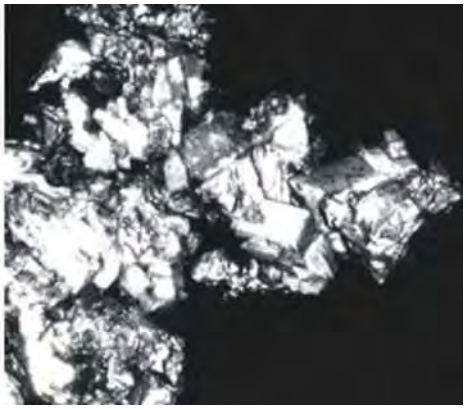
Non-centrosymmetric Metal Organic Frameworks (MOF) based on coordination of carbohydrates on alkaline metal ion represent an ideal category of compounds to plan functional materials with interesting second-order non-linear optics properties. Two MOFs obtained from fructose and calcium chloride, [Ca(C6H12O6)(H2O)2]Cl2 (1) and [Ca(C6H12O6)2(H2O)2]Cl2·H2O (2), have been synthetized in ethanol and by solid-solid interactions and have been characterized with X-ray diffraction and IR and RAMAN spectroscopy. The two compounds have also been studied with DFT theoretical calculations to investigate their relative stability and foresee their optical properties. Finally, the second harmonic generation (SHG) properties have been evaluated by SHG microscopy. It has been demonstrated that the coordination of fructose on the calcium ion causes an improvement of the SHG intensity with respect to the fructose itself and that there is a strictly correlation between the calculated dipole moment and the first static hyperpolarizability values and intensity of the SHG signal. Furthermore, the remarkable difference in the SHG intensity of the two compounds studied, suggests that this physical property can be "controlled" not only by tuning the composition of the system, but also by the disposition of the MOF's building units in the crystal. The metal-carbohydrate based MOFs analyzed in this work have a favorable combination of thermal and chemical stability, transparency, and second-order optical non-linearity and are thus potential candidates for applications in electro-optic devices.





Keywords: Second Harmonic Generation, carbohydrate-metal complex, Metal Organic Frameworks