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The peculiar SHG behavior of solid Co-, Ni- and Cu-porphyrinates

Porphyrins are the most studied heterocyclic macrocycle organic compounds for numerous applications, due to their optical properties and chemical stability. Among the optical properties, porphyrins show in solution interesting Non Linear Optical (NLO) Properties, i.e. Second (SHG) and Third (THG) Harmonic Generation [1,2]. At our knowledge, up to now in solid state the SHG properties of porphyrins or their derivatives were not investigated. Thus, we decided to investigate the SHG behaviour of three metal porphyrinates of formula M-TPP (M = Co, Cu and Ni, TPP = 5,10,15,20-tetraphenylporphyrine) in the solid state, that crystallize in the same acentric I-42d space group and are isomorphous.

We synthesized and characterized them and we measured the Second Harmonic Generation (SHG) response of powdered samples with a 1.907 μm pulsed laser radiation. For all the complexes, after few minutes of laser irradiation, a sudden enhancement of the intensity of the SH was observed. We attempted to understand the origin of this peculiar SHG behavior both through experimental analysis and theoretical calculations. In order to better correlate the second harmonic emission with the nature and structure of the materials, theoretical calculations were carried out with two different computational approaches: a model in which the crystalline fragment is represented as a nanoparticle (nanoparticle calculations) and a model in which the crystal is infinite and perfect (bulk calculations). In both cases the geometrical parameters were optimized and compared with the experimental XRD data; the first-order static hyperpolarizability and second-order susceptibility were also calculated and compared with the values obtained for the sucrose used as a reference. These results were compared with the experimentally SHG intensity ratios measured on the powders of the material with the method of Kurtz and Perry [3].

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