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### New 1D, 2D and 3D azido Mn, Cd and Zn complexes with magnetic and non-linear optical properties

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Supramolecular chemistry is concerned with weak interactions that occur between molecules, i.e. all non-covalent bonds, as well as weak coordination bonds. Such interactions are important in biological, magnetic and optical systems. Here we describe coordination compounds used as building blocks in crystal engineering. We present a number of supramolecular 1-D, 2-D and 3-D complexes of Mn<sup>II</sup>, Cd<sup>II</sup> and Zn<sup>II</sup> with the azido bridge as a networking agent. The versatility of the azide ligand affords chains with Mn<sup>II</sup> in which ferrimagnetic behavior is clearly observed for 1-D and 2-D Mn<sup>II</sup> systems with quinoline derivatives [Mn(H<sub>2</sub>O)(μ-N<sub>3</sub>)(N<sub>3</sub>(quinaz)<sub>2</sub>)<sub>n</sub> and [Mn(μ-N<sub>3</sub>)<sub>2</sub>(quinaz)<sub>2</sub>]<sub>n</sub> (quinaz = quinazoline) and [Mn(μ-N<sub>3</sub>)<sub>2</sub>(pyzamid)<sub>2</sub>]<sub>n</sub> and [Mn<sub>2</sub>(3-ampy)<sub>4</sub>(μ-N<sub>3</sub>)<sub>2</sub>(N<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub> (pyzamid = pyrazineamide and 3-ampy = 3-aminopyridine). The field of non-linear optics (NLO) is of considerable interest for many commercial applications. In particular, second-order harmonics generation, i.e. frequency doubling, which can be used in the conversion of red laser into blue laser light, is a desirable property. This requires a lack of inverse centre, an easy task in crystal engineering of coordination polymers with chiral components. We report the synthesis, spectral and structural characterization of some Cd<sup>II</sup> and Zn<sup>II</sup> complexes. The Kerr effect was studied as a property of the NLO materials for complexes [Cd<sub>3</sub>(nic)<sub>4</sub>(N<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>, [Zn(nic)(N<sub>3</sub>)]<sub>n</sub> (nic = nicotinate anion), [Cd(2,5-dmpyz)(N<sub>3</sub>)<sub>2</sub>]<sub>n</sub>, (dmpyz = dimethylpyrazine) and [Zn(bipy)(N<sub>3</sub>)<sub>2</sub>]<sub>n</sub> (bipy = 2,2'-bipyridine).

Keywords: supramolecular structures, metal-organic compounds, structure-function relationships in solids

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### Motion of inclusion gas molecules in clathrate hydrate observed by neutron powder diffraction

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Methane hydrate has attracted great interest as an energy resource after the discovery in the deep seabed as huge reservoirs of methane gas. Moreover, carbon dioxide hydrate is paid much attention as a storage medium of carbon dioxide gas to prevent the global warming. These clathrate hydrates are inclusion compounds in which the hydrophobic guest molecules exist in a host ice-framework called 'cage'. Their structural stabilities are deeply related with the physical properties of inclusion gases. In this study, we carried out neutron powder diffraction measurements of carbon dioxide and Xe deuterohydrates using the HRPD at JRR-3, JAEA. The diffraction data were analyzed by the combination of the Rietveld and the maximum entropy method (MEM) to clarify the motion of inclusion gases. The motions of carbon dioxide and Xe molecules in the small cages show the different manner from those in the large cages. These motions have small temperature dependences, in contrast to the methane hydrate case where the motion of methane molecules in the large cage shows large temperature dependence. Details on the motions of gas molecules in the hydrates are discussed.

Keywords: clathrate hydrate, neutron powder diffraction, MEM

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### Possible non-centrosymmetric structure of vaterite type yttrium orthoborate

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Yttrium and Lanthanide Orthoborates are promising candidates to be used in new-generation flat-panel display phosphors technologies. Despite extensive research on the Eu<sup>3+</sup> luminescence, in these compounds, fundamental questions remain unanswered regarding the relation between the vaterite type structure and the resulting Eu<sup>3+</sup> spectral features. High-resolution luminescence spectra do not permit to unambiguously distinguish between the alternatives of having either two or three cation sites in the structures, which are compatible with the crystal structures solved by single-crystal X-ray and neutron powder diffraction, respectively. Three samples: YBO<sub>3</sub>, Y<sub>0.85</sub>Eu<sub>0.15</sub>BO<sub>3</sub> and Y<sub>0.85</sub>Yb<sub>0.15</sub>BO<sub>3</sub> were prepared by solid-state reaction. We have undertaken an investigation, combining optical spectroscopy, second harmonic generation, X-ray powder diffraction and first-principles calculations, to correlate the optical features with the crystalline structure. Some remarkable results have been achieved: 1) all the samples show similar SHG intensities than the KDP and these increases with the doping concentration; 2) from Rietveld refinement and first-principles calculations we can distinguish between the hexagonal, orthorhombic and monoclinic symmetry. Moreover, doped samples are better refined in the acentric C<sub>2</sub> space group, thus, we can correlate the number of sites of Yttrium and point symmetry with the results obtained from Yb<sup>3+</sup> and Eu<sup>3+</sup> optical spectra. Complementary first-principles total-energy calculations also are shedding light in the structural analysis of the systems [1].

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