

MS37-P5 Testing soft donor-acceptor intermolecular interactions with high pressure.

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Weak intermolecular interactions have a fundamental role in diverse fields such as protein folding, enzymatic reactions, supramolecular chemistry, and crystal engineering. Hydrogen bonding interactions, among the most common interactions and ubiquitous in biological systems, have been therefore extensively studied. However, several non-hydrogen bonding interactions have received less attention and still need to be carefully investigated since they can also play a significant role in molecular self-assembly and single-crystal-to-single-crystal modifications (e.g. polymorphism and solid-phase chemical reactions). Among these, $\text{NO}_2 \cdots \text{NO}_2$ interactions are particularly interesting and somehow controversial; the nature of the interaction has been debated, but various results suggest that it is indeed attractive and comparable in energy to a weak hydrogen bond.

In this preliminary work, the crystal structure of 4-amino-4'-nitrophenyl was studied at different temperatures and different pressures, aiming to observe the behaviour of $\text{NO}_2 \cdots \text{NO}_2$ contacts under extreme conditions, when significant changes of stereo-electronic properties can occur due to the smaller volumes in which molecule are confined. A pressure-induced phase transition was observed above 1.6 GPa, associated with a severe rearrangements of the molecular packing, mainly driven by a $\text{NO}_2 \cdots \text{NO}_2$ interaction. Several high-pressure DFT calculations were also performed in order to select new possible study subjects in which the nitro-nitro distances may reach smaller values.

Keywords: high pressure, intermolecular interactions

MS37-P6 *Ab initio* crystal structure determination, thermal behaviour, and magnetic characterization of a new nickel coordination polymer based on carboxyethylphosphonic acid and 4,4'-bipyridine.

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The phosphonate type ligands have been widely used in the design and synthesis of new coordination polymers due to its strong ability to coordinate with transition and rare-earth metals under a set of different reaction conditions. These materials have a great interest not only due to their structural variety but also for their potential application in catalysis, gas storage, as magnetic materials, ion exchange, photoluminescent devices, intercalation chemistry, as sorbents, and in biomedical and biological process [1]. In this work we have obtained a crystalline powder aggregates of a new nickel coordination polymer $\text{Ni}_2(\text{HPPA})_2(4,4'\text{-bipy})_2(\text{H}_2\text{O})$ by hydrothermal synthesis, and their crystal structure has been *ab initio* determined from synchrotron powder data. The compound shows a layer structure in *bc* plane, with Ni atoms in two different environments. The loss of the coordinated water by heating leads to the apparition of an anhydrous phase, which remains stable when cooling down to room temperature. Synthesized material presents a paramagnetic behaviour until 10 K, showing some trends of being magnetically ordered below 2 K.

[1] a) Clearfield, A.; Demadis, K. (Eds.), *Metal Phosphonate Chemistry: From Synthesis to Applications*. RSC Publishing, Cambridge, UK, 2011; b) Brunet, E.; Colón, J. L.; Clearfield, A. (Eds), *Tailored Organic-Inorganic Materials*. John Wiley & Sons, New York, 2015.

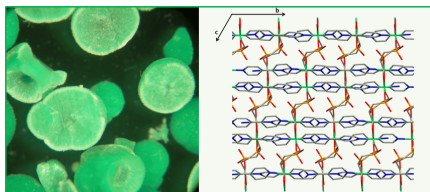


Figure 1. Morphology of the crystalline aggregates for the compound. (Zoom 1.6x) and packing diagram in *bc* plane, with a view of the 4,4'-bipyridine chains along *b*-axis, connected by the PPA ligands.