

crystallizes in monoclinic space group  $P2_1/n$ ,  $a=10.1737(2)$   $b=12.6997(3)$   $c=13.6447(3)$  Å,  $\beta=101.1920(10)^\circ$  and compound **2** crystallizes in monoclinic space group  $P2_1/n$ ,  $a=8.2966(3)$   $b=19.9133(6)$   $c=10.5516(3)$  Å,  $\beta=102.653(2)^\circ$ . In compound **1**, the cobalt center is hepta-coordinated by the three N atoms of the bdmpp ligand, two O atoms from one nitrito group and two O atoms from the other nitrito group. In compound **2**, nickel center is hexa-coordinated by the three N atoms of the bdmpp ligand, two O atoms from one nitrito group and the other nitrito group is bonded with an O(3) atom.

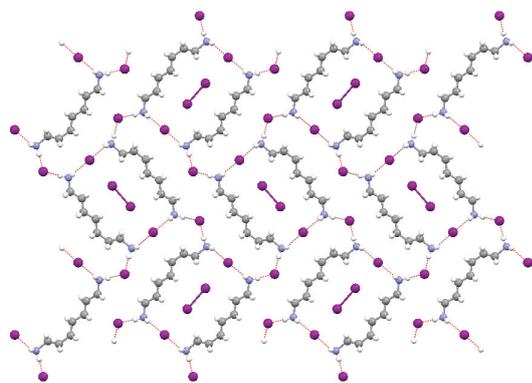
**Keywords:** transition-metal complexes; single-crystal analysis; thermal analysis

#### FA4-MS02-P18

**Iodine Inclusion in Heptane-1,7-Diammonium Diiodide Salts.** Charmaine van Blerk<sup>a</sup>, Gert J. Kruger<sup>a</sup>. <sup>a</sup>Department of Chemistry, University of Johannesburg, P O Box 524, Auckland Park, Johannesburg, 2006, South Africa. E-mail: [cvanblerk@uj.ac.za](mailto:cvanblerk@uj.ac.za)

Investigations into structure-property relationships and applications of *n*-alkyl-diammonium salts are of continued interest and form the basis of our continuing investigations of these materials since they have important applications. [1 – 4] We have previously investigated the dihalide salts of a variety of *n*-alkyl-diamines [5 – 7] and this current work focuses on the crystal chemistry of two diiodide salts of heptane-1,7-diamine.

Compound (**I**) is heptane-1,7-diammonium diiodide and compound (**II**) is heptane-1,7-diammonium iodine diiodide. Both compounds crystallize in an orthorhombic crystal system with compound (**I**) occupying the space group  $Pbca$  and compound (**II**) occupying the space group  $Pbcn$ . Significant differences exist in their crystal structures and we present and discuss their crystal chemistry in this work. The figure below shows the packing diagram of compound (**II**) viewed down the *c* axis. Both compounds produce an interesting array of three-dimensional hydrogen-bonding patterns consisting of multiple ring and chain motifs. Large ring motifs (a small inner ring with graph set  $R^2_4(25)$  and a large outer ring with graph set  $R^6_8(41)$ ) can be calculated for compound (**II**) and the ring motifs are evident in the figure below.



[1] Singh, G., Singh, C. P. & Mannan, S. M. *Thermochim. Acta*, **2005**, 437, 21 – 25. [2] Singh, G., Singh, C. P. & Mannan, S. M. *J. Hazard. Mater.*, **2006**, A135, 10 – 14. [3] Chen, F., Zhu, K., Gan, G. J., Shen, S. & Kooli, F. *Mat. Res. Bull.*, **2007**, 42, 1128 – 1136. [4] Takami, S., Sato, T., Mousavand, T., Ohara, S., Umetsu, M. & Adschiri, T. *Mater. Lett.*, **2007**, 61, 4769 – 4772. [5] van Blerk, C. & Kruger, G. J. *Acta Cryst.*, **2007**, E63, o342 – o344. [6] van Blerk, C. & Kruger, G. J. *Acta Cryst.*, **2007**, E63, o4289. [7] van Blerk, C. & Kruger, G. J. *Acta Cryst.*, **2008**, C64, o537 – o542.

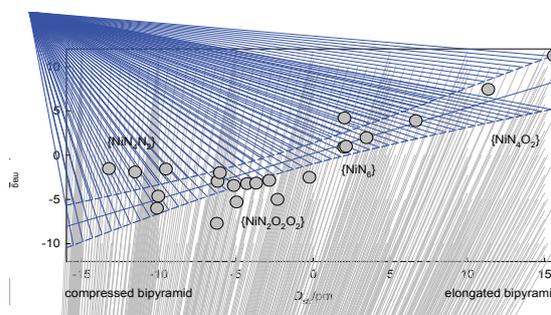
**Keywords:** *n*-alkyl-diammonium halide salts; single crystal X-ray diffractometry; iodine inclusion

#### FA4-MS02-P19

**Amagnetostructural D-correlation in Mononuclear Ni(II) Complexes.** Roman Boča. Institute of Inorganic Chemistry (FCHPT), Slovak University of Technology 812 37 Bratislava, Slovakia.

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A series of about 20 mononuclear Ni(II) complexes with a different donor set has been synthesized and structurally characterized. The metal-ligand distances (corrected to the heterogeneous donor set) have been used in obtaining a tetragonality parameter,  $D_{str}$ . In parallel, the SQUID magnetic data have been analyzed in terms of the spin Hamiltonian formalism, from which the axial zero-field splitting parameter  $D_{mag}$  (that characterizes the magnetic anisotropy) has been retrieved by a data fitting procedure. The values of  $D_{mag}$  correlate with  $D_{str}$  along a straight line and a rationalization of this novel magneto-structural D-correlation brings the crystal-field theory. Thus a rational tuning of the magnetic anisotropy becomes a realistic task.



[1] Boca, R.; Titiš, J., „Magnetostructural D-Correlation for Zero-Field Splitting in Nickel(II) Complexes“ in Coordination Chemistry Research Progress, Nova Science Publishers, New York, **2007**, pp.247-304.

**Keywords:** magnetic properties of molecules; structural correlation; nickel compounds

#### FA4-MS02-P20

**New Generation of Metal String Complexes: Strengthening Metal-metal Interaction via Naphthyridyl Group Modulated Oligo- $\alpha$ -pyridylamido Ligands.** Shie-Ming Peng<sup>a,b</sup>. <sup>a</sup>Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan (ROC). <sup>b</sup>Institute of