

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.

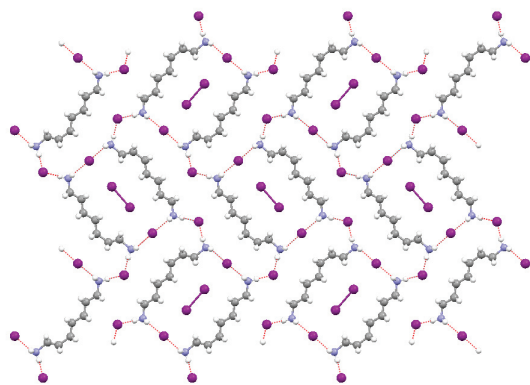
Keywords: transition-metal complexes; single-crystal analysis; thermal analysis

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Iodine Inclusion in Heptane-1,7-Diammonium Diiodide Salts. Charmaine van Blerk^a, Gert J. Kruger^a. ^aDepartment of Chemistry, University of Johannesburg, P O Box 524, Auckland Park, Johannesburg, 2006, South Africa. E-mail: 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.



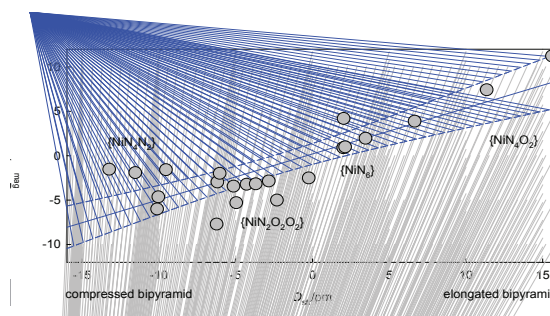
[1] Singh, G., Singh, C. P. & Mannan, S. M. *Thermochim. Acta*, **2005**, 437, 21 – 25. [2] Singh, G., Singh, C. P. & Mannan, S. M. *J. Hazard. Mater.*, **2006**, A135, 10 – 14. [3] Chen, F., Zhu, K., Gan, G. J., Shen, S. & Kooli, F. *Mat. Res. Bull.*, **2007**, 42, 1128 – 1136. [4] Takami, S., Sato, 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. E-mail: roman.boca@stuba.sk

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- α -pyridylamido Ligands. Shie-Ming Peng^{a,b}. ^aDepartment of Chemistry, National Taiwan University, Taipei, 106, Taiwan (ROC). ^bInstitute of

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To design new metal string complexes, several naphthyridyl group modulated oligo- α -pyridylamido ligands have been synthesized in the past five years. Because these ligands are less anionic than pyridylamido ligands, the resulting metal string complexes tend to form reduced mixed-valence $[\text{Ni}_2(\text{napy})_4]^{3+}$ dinuclear units which contain a delocalized unpaired electron and thus significantly enhance the conductance of metal string complexes. Furthermore, the asymmetric naphthyridyl group modulated oligo- α -pyridylamido ligands can stabilize the central heteronuclear or charge disproportionational metal frameworks, providing a plausible strategy to build inorganic molecular rectifiers.

1. Introduction
 - 1.1 Oligo- α -pyridylamido ligands and related metal string complexes
 - 1.2 Metal-metal bonding in the metal string complexes
 - 1.3 Single molecular conductance of the metal string complexes
2. Oligo- α -naphthyridylamido ligands and related nickel string complexes
 - 2.1 Synthesis and structures of the nickel string complexes
 - 2.2 Electron delocalization of the mixed-valence $[\text{Ni}_2(\text{napy})_4]^{3+}$ unit
 - 2.3 Single molecular conductance of the nickel string complexes
3. Oligo- α -naphthyridylpyridylamido ligands and related metal string complexes
 - 3.1 Linear hexanuclear metal string complexes
 - 3.2 Defective octanuclear nickel string complex
4. Asymmetric mixed-substituted ligands and related metal string complexes
 - 4.1 2-(Naphthyridylamino)-7-phenylamino-1,8-naphthyridine (H_2napy) ligand
 - 4.2 Novel charge disproportionational asymmetric heptanickel string complex
 - 4.3 Asymmetric 2-naphthyridylphenylamido ligand (Hnpy) and its heterometal string complexes
5. Summary

Keywords: metal-metal bonds; molecular wires; molecular switches

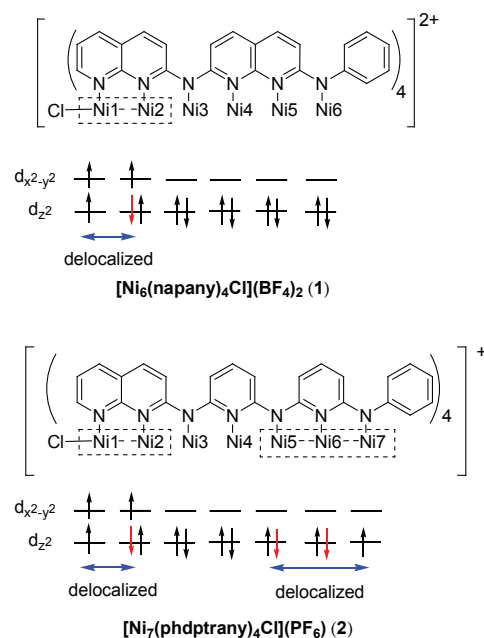
FA4-MS02-P21

Asymmetric Linear Nickel Metal String Complexes: A Manipulation of Electronic Structures through Supporting Ligands. Shao-An Hua^a, Isiah Po-Chun Liu^{a,b}, Shie-Ming Peng^{a,b}. ^aDepartment of Chemistry, National Taiwan University, Taipei, 106, Taiwan (ROC). ^bInstitute of Chemistry, Academia Sinica, Taipei, 115, Taiwan (ROC).

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Over the past decade, we have been showing that the combination of 1D linear metal framework with poly-

nitrogen ligands gives rise to the unique quadruple helix, which we describe as "metal string complexes"^[1]. Because the supporting ligands and the axial coordination play an essential role on altering the physical properties of these complexes, we explore the novel electronic structures by introducing asymmetrical ligand system. We present herein two newly synthesized hexa- and heptanickel metal string complexes $[\text{Ni}_6(\text{napy})_4\text{Cl}](\text{BF}_4)_2$ (**1**) and $[\text{Ni}_7(\text{phdptry})_4\text{Cl}]\text{PF}_6$ (**2**).^[2] Both of these complexes exhibit an asymmetric (4,0)- conformation, which the equatorial ligands align in the same direction with one axial ligand coordinated to the metal chain. Due to the differences of the supporting ligands, **1** and **2** reveal varied physical properties, clearly elucidated by means of crystal structures, magnetism, near-IR spectroscopy and DFT calculations. The complex **1** presenting only one MV $[\text{Ni}_2(\text{napy})_4]^{3+}$ dinuclear unit (napy = naphthyridyl group) within the metal framework, while an extending of MV units via an intriguing charge disproportionate mechanism is observed for complex **2**.



[1] C.-Y. Yeh, C.-C. Wang, C.-h. Chen and S.-M. Peng, in *Nano Redox Sites: Nano-Space Control and its Applications*, T. Hirao, Ed.; Springer: Berlin, **2006**, Chapter 5, pp. 85-117. [2] a) I. P.-C. Liu, C.-F. Chen, S.-A. Hua, C.-H. Chen, H.-T. Wang, G.-H. Lee and S.-M. Peng, *Dalton Trans.*, **2009**, DOI: 10.1039/b901675a; b) S.-A. Hua, G.-C. Huang, I. P.-C. Liu, J.-H. Kuo, C.-H. Jiang, C.-L. Chiu, C.-Y. Yeh, G.-H. Lee and S.-M. Peng, *Chem. Eur. J.*, submitted.

Keywords: metal-metal bonds; mixed-valence compounds; electronic structure

FA4-MS02-P22

Syntheses and Studies of Linear Metal String Complexes: $[\text{Ni}_{10}(\mu_{10}\text{-bdpdany})_4(\text{NCS})_2](\text{PF}_6)_2$ and $[\text{Ru}_2\text{Ni}_2(\text{DAniDANy})_3(\text{OAc})_2\text{Cl}]$. Jau - Huei Kuo^a, Gin-Chen Huang^a, Shie-Ming Peng^{ab}. ^aDepartment of