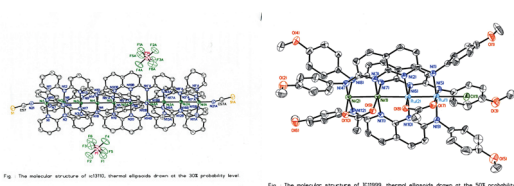


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Our group was devoted to the research of metal string complexes in past decades. We believe that the thinnest metal wire could be applied to practical applications in molecular electronics in future. We successfully synthesized two kinds of ligand in order to extend the study of metal strings. First, the new decametal string complex  $[\text{Ni}_{10}(\mu_{10}\text{-bdpdany})_4(\text{NCS})_2](\text{PF}_6)_2$  was successfully synthesized with  $\text{H}_4\text{bdpdang}$  ligand. The crystal structure of  $[\text{Ni}_{10}(\mu_{10}\text{-bdpdany})_4(\text{NCS})_2](\text{PF}_6)_2$  shows that all of the  $\text{bdpdany}^{4-}$  ligands bind metal in all-syn conformation and the X-ray structural studies reveal the internal Ni-Ni bond distance is ca. 2.36~2.23 Å. Second, the heteronuclear  $[\text{Ru}_2\text{Ni}_2(\text{DAniDANy})_3(\text{OAc})_2\text{Cl}]$  complex was successfully synthesized with  $\text{H}_2\text{DAniDANy}$  ligand. The crystal structure of  $[\text{Ru}_2\text{Ni}_2(\text{DAniDANy})_3(\text{OAc})_2\text{Cl}]$  is shown in Figure 1b. Ru(1)-Ru(2) is about 2.288(1) Å. Ru(1)-Cl is 2.469(2) Å. Ru-N distances are 2.04-2.09 Å. Ru(2)-Ni(1) is 2.469(1) Å. This distance is close enough to have some overlap between Ru and Ni. Magnetic study shows it has three unpaired electrons. IVCT band at 890 nm indicates there exists an unoccupied  $\delta^*$  which is similar to  $\text{Ru}_2$  dimer. DFT study shows that the three magnetic orbitals are essentially  $\text{Ru}_2$  based.  $\text{Ru}_2$  and  $\text{Ni}_2$  may have weak bonding interaction.



**Fig. 1** The crystal structures of  $[\text{Ni}_{10}(\mu_{10}\text{-bdpdany})_4(\text{NCS})_2](\text{PF}_6)_2$  and  $[\text{Ru}_2\text{Ni}_2(\text{DAniDANy})_3(\text{OAc})_2\text{Cl}]$ .

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**Keywords:** metal-metal bonds; crystallography; magnetic properties

#### FA4-MS02-P23

**Insight into Crystal Structure/Optical Properties Relationships of New N-Salicylidene Anils.** Bernard Tinant<sup>a</sup>, François Robert<sup>a</sup>, Anil D. Naik<sup>a</sup>, Yann Garcia<sup>a</sup>. <sup>a</sup>Unité de Chimie Structurale et des Mécanismes Réactionnels et Unité de Chimie des Matériaux Inorganiques et Organiques, Département de Chimie, Université Catholique de Louvain, Place L. Pasteur 1, B-1348 Louvain-la-Neuve, Belgium.  
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N-salicylidene aniline derivatives are highly versatile thermo- and photochromic molecules [1]. These are actively studied for many applications like non linear optics [2], biological activities [3], information storage and display

[4], etc. Thermo and photochromism occurring in the solid state thanks to reversible equilibria between the uncoloured *enol*, the yellow *cis-keto* and the red *trans-keto* forms [1] are the main interests of these compounds. All derivatives are described as thermochromic but only a few of them are photochromic. Many authors stress the importance of crystal packing [5] to explain these properties but the molecular environment is also to be considered [6]. Crystallographic study of N-salicylidene aniline derivatives is essential for the understanding of molecular properties in solution or in solid state. In this work, we have observed that the dihedral angle between aromatic rings and the crystal packing are not sufficient to predict the photochromism behaviour of the compounds [7]. This is clearly seen with the N-salicylidene 4-aminopyridine (L4) and 2-(3,5-bis(pyridin-2-yl)-1,2,4-triazole-4-ylimino-methyl)-phenol (ABS). L4, a highly twisted molecule, present an open structure with large intermolecular distances and weak CH- $\pi$  and  $\pi\pi$  stacking interactions. Photo-isomerisation to the *trans-keto* form should be easier thanks to the crystal packing. However, L4 is only thermochromic. In contrast, ABS crystal is formed with highly twisted molecules, packed very closely with strong supramolecular interactions ( $\pi\pi$  stacking) but is only photochromic. This observation clearly disagrees with reported conclusions [5]. Finally, a novel interesting molecular conformation has been discovered with the N-salicylidene 4-amino-1,2,4-triazole (Hsaltrz) which is packed as supramolecular *zig-zag* double chains.

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**Keywords:** supramolecular chemistry; crystal structure; optical properties

#### FA4-MS02-P24

**Cation and Ligand Roles in the Coordination of Fe<sup>III</sup> Bisdithiolene Complexes.** Isabel Corderio Santos<sup>a</sup>, Ana Isabel S. Neves<sup>a</sup>, Dulce Belo<sup>a</sup>, Manuel Almeida<sup>a</sup>. <sup>a</sup>Dept. Química, I.T.N./CFMUL, P-2686-953, Sacavém, Portugal.

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Aiming at a better understanding of the role of the cation versus the role of the ligand in the coordination geometry of Fe<sup>III</sup> bisdithiolene complexes we have been exploring either new  $[\text{Fe}^{\text{III}}(\text{qdt})_2]^-$  salts (qdt=quinoxalinedithiolate) with different cations or new iron bisdithiolates complexes, such as  $[\text{Fe}(\alpha\text{-tpdt})_2]$  ( $\alpha\text{-tpdt}$ =2,3-thiophenedithiolate). At variance with the large diversity of coordination geometries and oxidation states of bisdithiolene complexes with most metals, the iron complexes with these ligands have been essentially restricted to one stable oxidation state, Fe(III), and until quite recently all were found to adopt in solid state the same square pyramidal, 4+1, coordination geometry due