systems are tris(diketonate) coordination compounds of trivalent metals. This was noticed as early as 1926 when has been noted that the crystal structures of trivalent metal pentane-2,4-dionato complexes of various metals appear to be grouped in several isomorphous series [2]. If the metal atom is coordinated by asymmetrical diketonate, two different isomers (facial and meridial) are possible.

Our work concentrated on compounds where trivalent metals are coordinated by 1-phenylbutane-1,3-dionato ligands which were studied by single crystal X-ray diffraction and thermal analysis. The meridial complexes of iron(III), manganese(III), chromium(III) were already reported to be isomorphous based on their powder diffraction patterns [3]. We have shown that thay crystallize in the monoclinic system, space group  $P2_1/c$ . The only facial isomers which could be isolated where those of chromium(III) and cobalt(III) complexes. They were both found to crystallize in two pseudopolymorphic modifications. Pure compounds crystallize in the space group P-1 with two molecules in the asymmetric unit. The crystal structures of the chromium and cobalt compounds are almost identical. Under same crystallization conditions, both compounds can also crystallize as hydrates. The hydrates crystallize in the space group R-3with 12 molecules per unit cell. The two symmetrically independent molecules in the structure differ in the mode of hydratation. As is the case with the triclinic modifications, the trigonal modifications of both chromium and cobalt compounds are almost perfectly isostructural

 A. Kálmán, L. Párkányi, G. Argay, Acta Cryst. (1993) B49, 1039.

[2] W. T. Astbury, Proc. Roy. Soc. (1926) 28, 313.

[3] R. C Fay, T. S. Piper, J. Am. Chem. Soc. (1962) 84, 2303.

## MS13 P08

Naphthyridines as building blocks: the helix structure of 2-N-acetylamino-7-methyl-1,8-naphthyridine. Laura Torre-Fernández<sup>a</sup>, Santiago García-Granda<sup>a</sup>, Shyamaprosad Goswami<sup>b</sup>, <sup>a</sup>Departamento de Química Física y Analítica, University of Oviedo, (Spain). <sup>b</sup>Departament of Chemistry, Department of Chemistry, Deemed University, West Bengal (India). E-mail: ltf@fq.uniovi.es

## Keywords: hydrogen bonding, supramolecular, Naphthyridines

Multiple hydrogen-bonded assemblies in biological systems are important for the formation of the DNA double helix [1], [2] and protein helical structures [3]. It is interesting to further explore the possibility of multiple hydrogen-bonding in naphthyridines stabilizing the catemers especially those giving rise to helical structures [4].

The 1,8-naphthyridine system functionalized at positions 2 and/or 7 are promising for supramolecular architectures although they are not often used. We report the crystal molecular structure including the supramolecular selfassembly of one of this naphthyridines, 2-N-acetylamino-7-methyl-1,8-naphthyridine with helical structure formed by both helices of opposed chirality, P and M, this could lead to helix structures. Interestingly, the terminal points i.e. the amide proton (N-H) and ring nitrogen (N3) take part in hydrogen bonding and a helical structure result for this compound. Non-classical hydrogen bond interactions are shown in between N2···H1-C11 and N2···H01-C1. Other two normal type of hydrogen bonds are found between N1-H2···N3 and N3···H2-N1 which are the key bond in the formation of single helical structure. An interlayer interaction is found between the interaction of C5-H6···O1.



Fig.1. View illustrating the selfassembling hydrogen-bonded helices.

[1] Yoder, M. D.; Keen, N. T.; Jurnak, F. Science, 1993, 260, 1503.

[2] Raetz. C. H. R.; Roderick, S. L. Science, 1995, 270, 997.

[3] Strobel, S.; Doucette-Stamm, L.; Riba, L.; Housman, D.; Dervan, P. *Science*, 1991, 254, 1639.

[4] Goswami, S. P.; Mukherjee, R.; Mukherjee, R; Jana, S.; Maity, A. C. A.; Adak, K. Molecules, 2005, 10, 929.

## MS13 P09

Synthesis and Characterization of New Cerium and Chromium Compounds Barbara M. Casari<sup>a</sup>, <u>Vratislav</u> <u>Langer<sup>b</sup></u>, <sup>a</sup>Department of Chemistry, Inorganic Chemistry, Göteborg University, SE–412 96 Göteborg, Sweden. <sup>b</sup>Environmental Inorganic Chemistry, Department of Chemical and Biological Engineering, Chalmers University of Technology, SE–412 96 Göteborg, Sweden. E-mail: casari@chem.gu.se

## Keywords: Mixed valence, Cerium compounds, Chromium compounds

Syntheses and structural characterization of the compounds  $\alpha$ - and  $\beta$ -Ce(SO<sub>4</sub>)<sub>2</sub>:4H<sub>2</sub>O, Ce<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>:4H<sub>2</sub>O,  $\beta$ -Ce<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>:8H<sub>2</sub>O, K<sub>5</sub>Ce<sub>2</sub>(SO<sub>4</sub>)<sub>6</sub>:H<sub>2</sub>O, K<sub>2</sub>Ce(SO<sub>4</sub>)<sub>3</sub>:H<sub>2</sub>O, K<sub>5</sub>Na[Ce<sub>2</sub>(SO<sub>4</sub>)<sub>6</sub>],CrCe(III)<sub>7</sub>Ce(IV)<sub>6</sub>(HSO<sub>4</sub>)<sub>6</sub>(SO<sub>4</sub>)<sub>21</sub>:75H<sub>2</sub> O K<sub>6</sub>[Ce(HSO<sub>4</sub>)<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>]:H<sub>2</sub>O, A<sub>2</sub>[CrCl<sub>5</sub>(H<sub>2</sub>O)], (A = NH<sub>4</sub>, K, Rb, Cs), NH<sub>4</sub>Cr(CrO<sub>4</sub>)<sub>2</sub> and K<sub>2</sub>CrSO<sub>7</sub> are presented. The crystal structures have been determined from single crystal X-ray data and the thermal behaviours have been studied by TG, DSC and X-ray powder thermodiffractometry. The decomposition of Ce(SO<sub>4</sub>)<sub>2</sub>, into the final product CeO<sub>2</sub>, proceeds through intermediate xCeO<sub>2</sub>·yCe(SO<sub>4</sub>)<sub>2</sub> species. However, during the oxidative decomposition of Ce<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> into CeO<sub>2</sub>, small amount of CeO(SO<sub>4</sub>) is produced.

The four salts of the catalytically active  $[CrCl_5(H_2O)]^{2-}$ complex are prepared by different methods and reaction pathways are suggested. These compounds are composed of  $[CrCl_5(H_2O)]^{2-}$  units connected by O–H····Cl hydrogen bonds and a counter ion framework. Further, for the first time, a mixed-valence chromium oxide has been synthesized starting from  $CrO_3$  in water solution. The reduction of the Cr(VI) into Cr(III) is presumably promoted by the oxidation of Ce(III). Among the mixed-