



Figure 1. The molecular structure of the complex with displacement ellipsoids drawn at the 30% probability level and hydrogen atoms have been omitted for clarity.

Keywords: N-heterocyclic carbene, Ir(I) complex, benzimidazol-2-ylidene, crystal structure

MS30-P14 Ligand type and synthetic approach induced variability of supramolecular topologies of $[\text{Ni}_4\text{L}_4(\text{ROH})_4]$ AND $[\text{Ni}_4\text{L}_4(\text{ROH})_X(\text{R}'\text{OH})_Y; X+Y = 4]$

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The synthesis of polynuclear cluster compounds of the Mn, Fe, Ni, V and Co or mixed metals represents a number of challenges. Often it is difficult to predict the exact cluster structure due to potentially variable outcomes of self-assembly process. Owing to a wide range of their potential applications, e.g. in data storage, memory devices, switches and sensors, considerable attention has been devoted to the targeted synthesis of such systems. The impact of reversible release and reabsorption of both coordinated and uncoordinated solvent molecules on the cluster properties is well documented in the literature.¹ These processes are accompanied by the structural changes related to a cleavage/formation of the coordination bonds.^{2,3} Among different cluster types that can exhibit those features, cubane-like clusters with $[\text{Ni}_4(\mu_3\text{-O})_4]$ core are especially well studied class. The cubane-like core of nearly all investigated tetranuclear Ni(II) complexes consists of four identical $\mu_3\text{-O}$ bridges originating from -OH or -OR moieties. The symmetry of $[\text{Ni}_4\text{O}_4]$ core and the differences in the $\text{Ni}-\mu_3\text{-O}-\text{Ni}$ angles often have a decisive role in establishing intramolecular magnetic interactions. $[\text{Ni}_4\text{L}_4(\text{sol})_4]$ type of complexes can undergo reversible exchange of the coordinated solvent molecules (MeOH vs. H_2O).⁴ Although the structural alterations induced by such solvent exchange were subtle, substantial changes of the physical and chemical properties have been established. This study unveiled novel synthetic aspects and interesting structural features of a new family of Ni(II) compounds based on cubane-like clusters. Depending on reaction conditions different cubane-like clusters of the type $[\text{Ni}_4\text{L}_4(\text{ROH})_4]$ and $[\text{Ni}_4\text{L}_4(\text{ROH})_2(\text{R}'\text{OH})_2]$ (H_2L = tridentate Schiff base ligand,

N -(2-hydroxy-5-methylphenyl)salicylideneimine, $\text{R} = \text{-CH}_3, \text{-C}_2\text{H}_5, \text{-C}_3\text{H}_7, \text{-C}_4\text{H}_9, \text{ i } \text{-C}_5\text{H}_{11}$) were isolated (Fig.1). The various supramolecular phenomena such as polymorphism, conformational isomorphism and synmorphism were established. These phenomena will be discussed in detail on the basis of structure-property relationships. ¹ H. Zheng-Ming, X.-M. Zhang, *Dalton Trans.* 2011, 40, 2092–2098. ² E.-C. Yang, et. al., *Polyhedron* 2003, 22, 1727–1733. ³ M. Moragues-Cánovas, et. al., *Eur. J. Inorg. Chem.* 2004, 2219–2222. ⁴ A. Das, et. al., *Inorg. Chem.* 2012, 51, 8141–8149.

Keywords: cubane-like clusters $[\text{Ni}_4\text{L}_4(\text{sol})_4]$; solv = ROH, tridentate Schiff base ligand, synthesis, supramolecular topologies