

Raman Study of Nickel(II) Complexes with 6-Methylpicolinic Acid

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The first **(1)** nickel(II) complex with 6-methylpicolinic acid was prepared by mixing of 6-methylpicolinic acid and nickel(II) nitrate hexahydrate solutions, while the second **(2)** complex was prepared by recrystallization of **(1)** from DMF solution [1]. Pseudopolymorphism of these two complexes was identified and characterized by means of X-ray, Raman, IR, calorimetric and DFT methods. X-ray diffraction study discovered two structures differing mainly in crystal packing due to the presence **(1)** or absence **(2)** of hydrated water molecules (see Fig. 1; **(2)** is isostructural with Co(II) complex [2]).

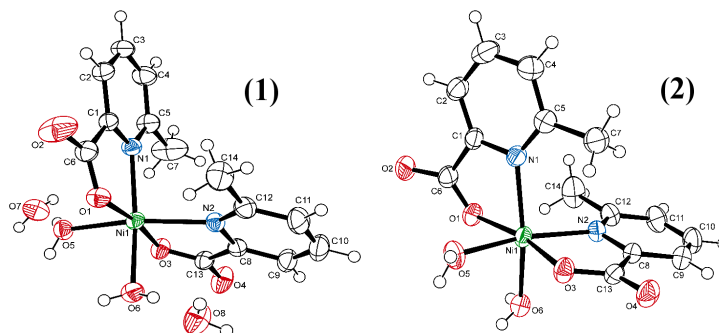


Fig. 1: ORTEP-3 drawings of $[\text{Ni}(6\text{-Mepic})_2(\text{H}_2\text{O})_2]\cdot 2\text{H}_2\text{O}$ **(1)** and $[\text{Ni}(6\text{-Mepic})_2(\text{H}_2\text{O})_2]$ **(2)**.

Raman spectroscopy of both $[\text{Ni}(6\text{-Mepic})_2]$ complexes confirmed that difference of two structures is correlated with the presence of water molecule that appears incorporated in the solid structure across two different hydrogen bonds of weak and medium strengths.

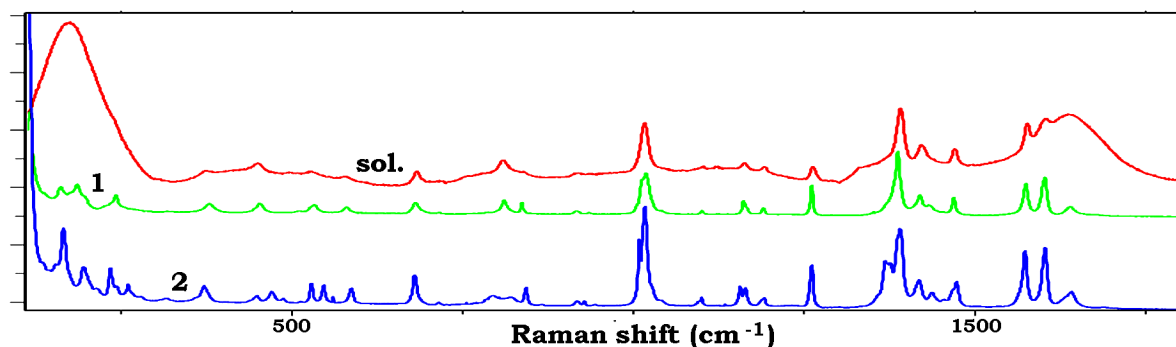


Fig. 2: Fingerprint region of Raman spectra of the solution and both Ni complexes **(1)** and **(2)**.

All bands observed for crystalline matter and for the solution, together with the assignment based on other similar complexes and methylpyridine [3], verify X-ray study results.

[1] B.M. Kukovec *et al*, International School of Crystallography, 39th Course, Erice, Italy, 2007, Lecture Notes and Poster Abstracts, Part 2, p. 626.

[2] R. March *et al*, Inorg. Chim. Acta 353 (2003) 129-138.

[3] J.F. Arenas, I. López Tocón, J.C. Otero, J.I. Marcos, J. Mol. Struct. 476 (1999) 139.