Poster

Synthesis and crystal structure analysis of a Ni(II) complex with Schiff base 2,6-diacetylpyridine-adamantane-1-carbohydrazide

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The interesting aspect of research on Schiff bases derived from 2,6-diacetylpyridine lies in their versatile coordination modes, which is is also confirmed by the search of the Cambridge Structural Database. This search contains structures of over 2500 of mentioned Schiff bases and their complex compounds. Among them, there are 133 nickel(II) complexes[1]. This work describes the synthesis and structural characterization of a new Ni(II) complex with this type of Schiff base.

In the reaction of a warm suspension of ligand 2,6-diacetylpyridine-adamantane-1-carbohydrazide in methanol and a warm acetone solution of nickel(II)-trifluoroacetate, in the presence of lithium-acetate, in molar ratio 1:1:1, the red stick crystals of new complex, $[Ni_2((Ad)_2dap–H)_2]\cdot MeOH$, was obtained.

The coordination is primarily assumed by the comparison of IR spectrum of the complex with the spectrum of the ligand. The molar conductivity value of this complex (Λ_M=2.66 S cm^2 mol^{-1} – in methanol) indicates that the obtained compound is non-electrolyte. The Schiff base in the newly synthesized compound has a role of N3O2 pentadentate ligand. One azomethine atom and one carbonyl oxygen atom are coordinated to one Ni(II), while the other azomethine nitrogen and carbonyl oxygen donor atoms of the same ligand molecule are coordinated to the neighboring metal atom in this dinuclear complex. The pyridine nitrogen atom is bonded for both metal atoms, and represents a bridge between them in the described structure. In this way, eight five-membered and one four-membered metallocycles are formed (Fig. 1). Both metal centers are located at octahedral environment of the ligand donor atoms.

The distance between two metal centers is 3.1147(7) Å. The bond length of the metal–ligator atom bond is in the range 1.960(3) – 2.437(3) Å, with the metal atom being the furthest from pyridine nitrogen atom, while the azomethine nitrogen atoms are the best electron donors in the complex $[Ni_2((Ad)_2dap–H)_2]\cdot MeOH$.

The structure is additionally stabilized by a hydrogen bond formed between the methanol oxygen atom as a hydrogen donor and the carbohydrazide oxygen atom in the role of a hydrogen acceptor (the value of the O3–H10–O1 angle is 158.57^0).

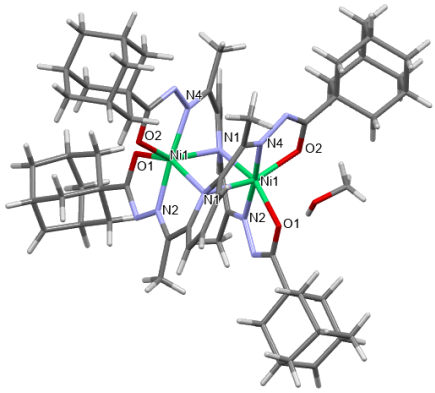

Figure 1. The molecular structure of the complex $[Ni_2((Ad)_2dap–H)_2]$

*[1] Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). Acta Crystallogr. B Struct. Sci. Cryst. Eng. Mater., **72**, 171.*

The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants No. 451-03-66/2024-03/ 200125 & 451-03-65/2024-03/200125)