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Jana Pisk, Biserka Prugovečki, Tomislav Jednačak, Predrag Novak, Višnja Vrdoljak

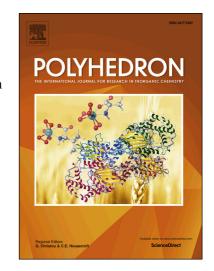
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## **ACCEPTED MANUSCRIPT**

# Intriguing binding modes of tetradentate pyridoxal derivatives to molybdenum centre

Jana Pisk, Biserka Prugovečki, Tomislav Jednačak, Predrag Novak, Višnja Vrdoljak<sup>a,\*</sup>

#### **ABSTRACT**

The Schiff base pdxen ligands ( $H_2py_2en = N,N'$ -ethylenebis(pyridoxylideneimine and  $H_2py_2pren = N,N'$ -prophylenebis(pyridoxylideneimine)) were found to form readily by the mechanochemical synthesis from their corresponding diamine and pyridoxal. Reduction of the Schiff bases with NaBH<sub>4</sub> yielded reduced pdxan ligands ( $H_2Rpy_2en = N,N'$ -ethylenebis(pyridoxylamine) and  $H_2Rpy_2pren = N,N'$ -prophylenebis(pyridoxylamine)). A dinuclear molybdenum(VI) complex with the bridging pdxen ligand [ $\{MoO_2\}_2(\mu$ -py<sub>2</sub>en)(OMe)<sub>2</sub>(MeOH)<sub>2</sub>]·3MeOH (**1·3MeOH**), and mononuclear complexes with the pdxen ligand [ $MoO_2(py_2pren)$ ] (**3**), as well as with the pdxen ligands: [ $MoO_2(Rpy_2en)$ ] (**2**) and [ $MoO_2(Rpy_2pren)$ ] (**4**) were prepared and characterized. Significant differences in the coordination of the Schiff base ligands were found as a consequence of chain length and ligand flexibility. Complexes **1–4** were obtained either by the reaction of [ $MoO_2(acac)_2$ ] or [ $Mo(CO)_6$ ] with the corresponding ligands. Crystal and molecular structures of complexes **1·3MeOH**, **2** and **3** were determined by the single crystal X-ray diffraction method. All complexes were characterized by microanalysis, FT-IR, NMR, UV, thermogravimetric analysis and powder X-ray diffraction method.

**Keywords:** pyridoxal; molybdenum(VI) complexes; tetradentate ligand; Schiff base; bridging ligand; coordination modes

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