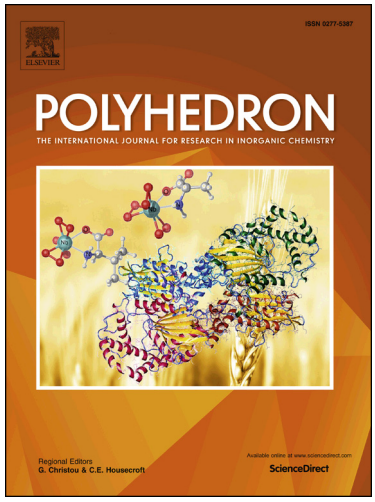


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# A comparison of ligand behaviors and interactions during supramolecular assembly using molecular dynamics simulation: synthesis, solid state and solution studies of two Ni(II) compounds

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**ABSTRACT**

Two nickel(II) supramolecular compounds $[Ni(H_2O)_6](4\text{-apyH})_2[Ni(2,6\text{-pydc})_2]_2.4H_2O.2EtOH$ (**1**) and $[Ni(2,3\text{-pydcH})_2.2H_2O]$ (**2**) (where 4-apy = 4-aminopyridine, 2,3-pydc$H_2$ = 2,3-pyridinedicarboxylic acid and 2,6-pydc$H_2$ = 2,6-pyridinedicarboxylic acid) were structurally compared in their solid state and solution forms. While the 2,6-pydc ligand in compound **1** uses both its carboxylate groups for coordination to nickel(II), the 2,3-pydc ligand in compound **2** binds through only one of the carboxylate groups, and the second carboxylate group which is expected to bind to another Ni(II) atom, does not coordinate to the metal. Using molecular dynamics simulations, it was shown that differences in ligands' binding affinities could be correlated to different behaviors and interactions during proton-transfer assembly of these ligands.

**Keyword:** supramolecular compound; molecular dynamics simulation; crystal structure; H-bond; solution studies

## Introduction