

## Hydrothermal synthesis, X-ray structure and DFT and magnetic studies of a $(\text{H}_2\text{SiW}_{12}\text{O}_{40})^{2-}$ based one-dimensional linear coordination polymer.

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### Streszczenie

In this paper, we report the synthesis and characterization of a novel hybrid with an inorganic–organic structure formulated as  $[[\text{Nd}_2(\text{L}^1)_2(\text{L}^2)(\text{H}_2\text{O})_7][\text{H}_2\text{SiW}_{12}\text{O}_{40}]]_n \cdot 4\text{H}_2\text{O}$  (**1**), in which  $\text{HL}^1$  = nicotinic acid and  $\text{H}_2\text{L}^2$  = 2-hydroxynicotinic acid. Interestingly,  $\text{L}^1$  and  $\text{L}^2$  are generated from an *in situ* transformation of the original ligand, pyridine-2,3-dicarboxylic acid under hydrothermal conditions. Structural analysis showed that this compound is a one-dimensional linear coordination polymer constructed from a repetition of the Keggin anion as a bidentate bridging ligand and one propeller-like dinuclear neodymium complex. Furthermore, in the packing arrangement, hydrogen bonds and anion– $\pi$  interactions connect the adjacent chains to extend the structure into a 3D architecture. The magnetic properties of this compound have also been studied by measuring its magnetic susceptibility in the temperature range 1.8–300 K. We also analyzed the coordination ability of the  $\text{SiW}_{12}$  Keggin anion in the reported structures up to now. Finally, we have performed a DFT computational study on the noncovalent anion– $\pi$  interactions between the Keggin anion and the aromatic ligands coordinated to Nd

### Adres publiczny

<http://dx.doi.org/10.1039/c4dt03950e>

### Strona internetowa wydawcy

<https://www.rsc.org/>

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/liOINob>.