Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information

A New Molybdenum(V) Nickel Phosphate Based on Divacant $[H_{30}(Mo^{V}_{16}O_{32})Ni_{14}(PO_4)_{26}O_2(OH)_4(H_2O)_8]^{12-}$ Wheel

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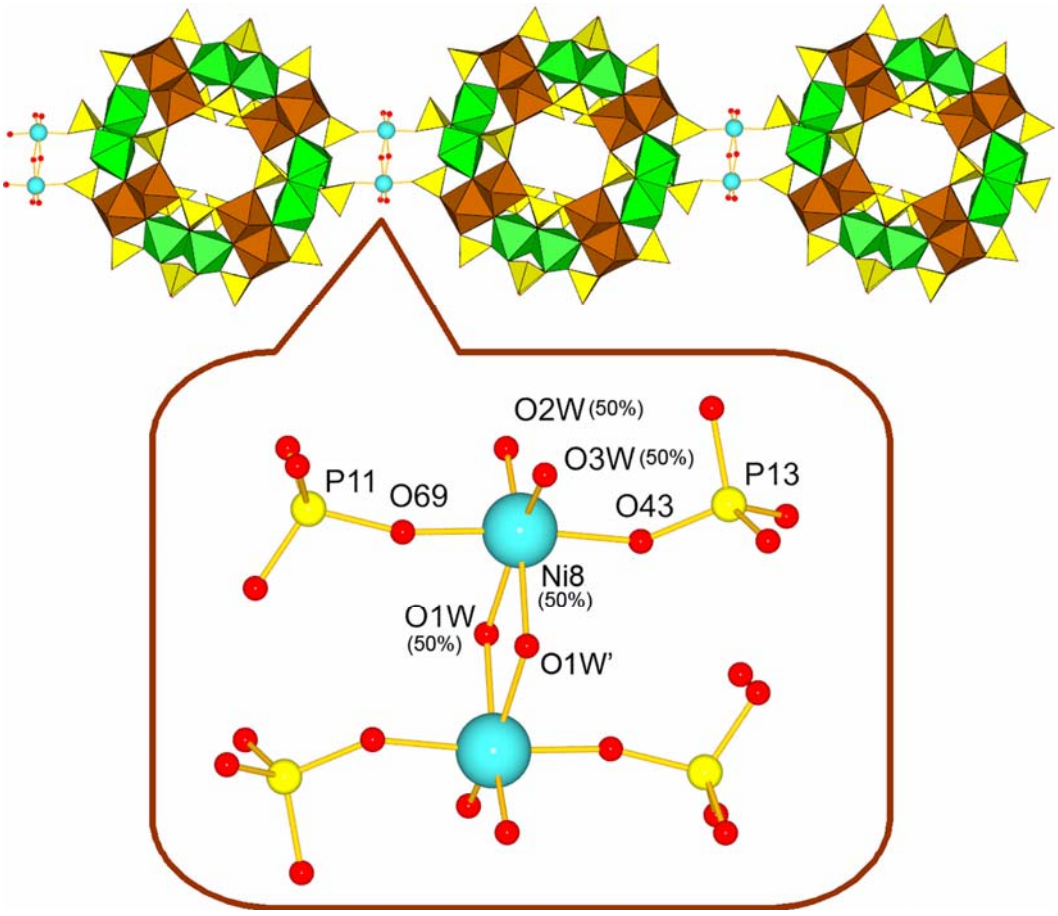

Fig. S1 View of 1-D chainlike structural feature of **1** composed of the wheel-type polyoxoanions and the $[Ni(H_2O)_3]^{2+}$ linkers. In such a linker, the Ni8 atom and its three coordinated water molecules all exhibit a 50% of site-occupancy disorder**.** The occupancies are shown in the parentheses. Color code: brown octahedra, $\{MoO_6\}$; green octahedra, $\{NiO_6\}$; yellow tetrahedra, $\{PO_4\}$, blue ball, Ni center; yellow ball, P atom; red ball, O atom. The bond distances of Ni(8)-O are in the range of 1.954(6)~2.123(2) Å.

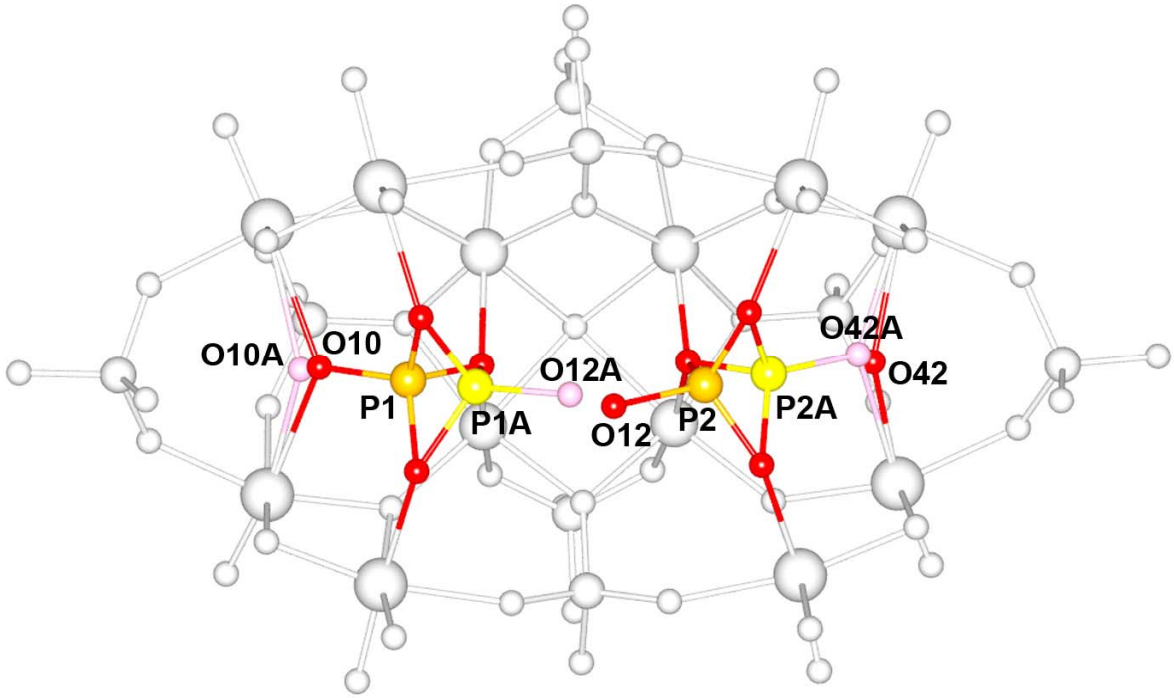

Fig. S2 View of the two-fold disordered $\{P(1)O_4\}$, $\{P(2)O_4\}$, O10 and O42 units in the polyoxoanion of **1**. The orange $\{P(1)O_4\}$, $\{P(2)O_4\}$ units and the red O10 and O42 linker possess 82% site occupancies, while the yellow $\{P(1A)O_4\}$ and $\{P(2A)O_4\}$ units and the pink O10A and O42A linkers possess 18 % site occupancies, respectively.

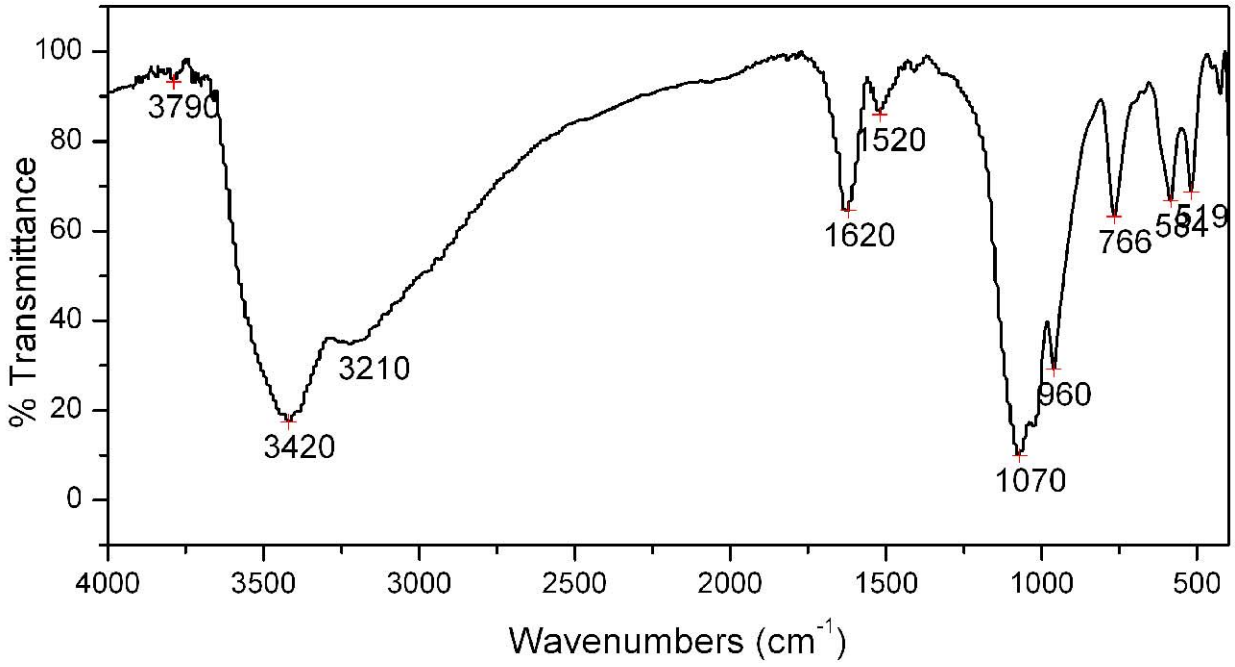

Fig. S3 IR spectrum of **1**

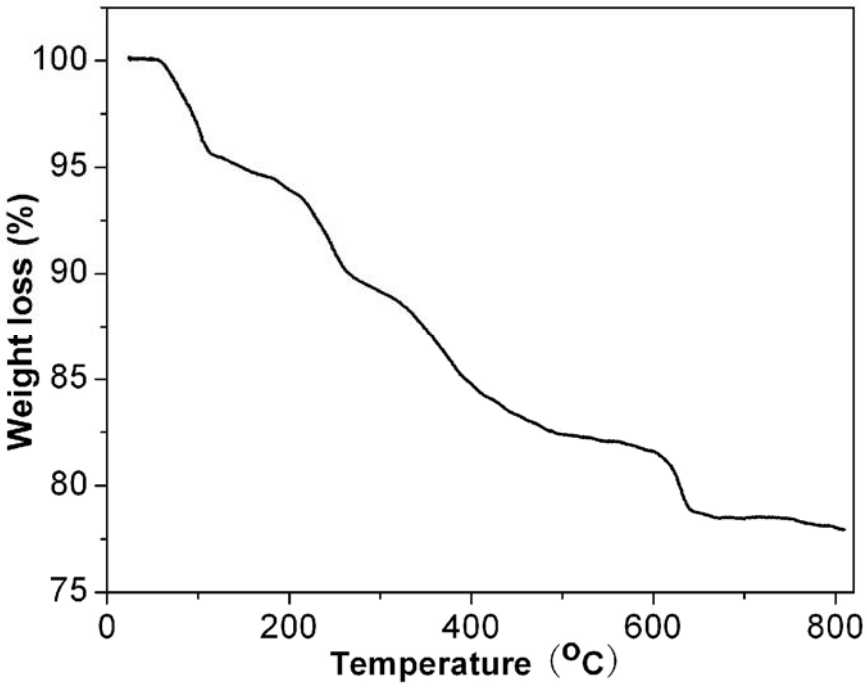

Fig. S4 TG curve of **1**

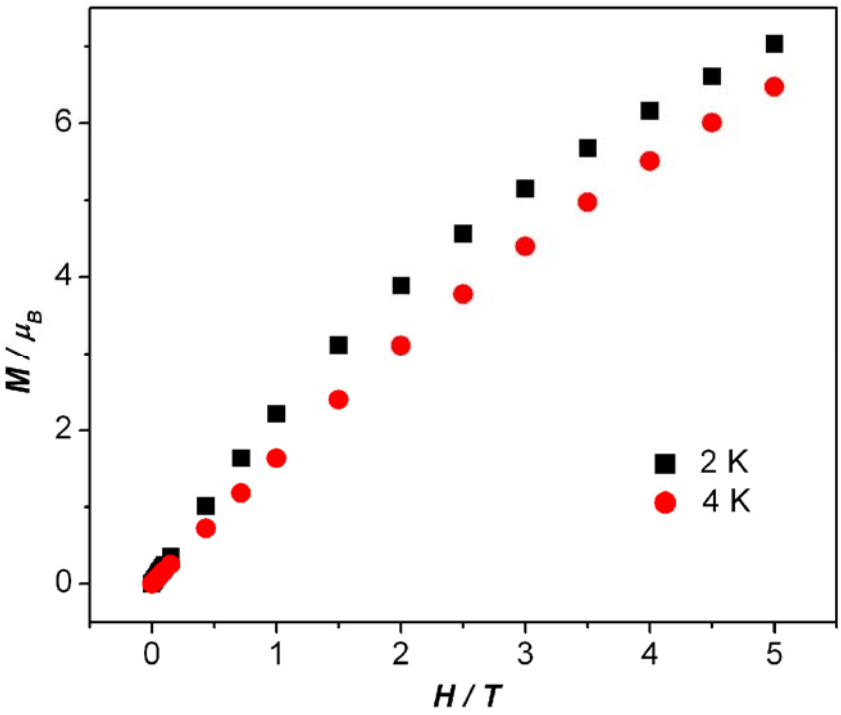

Fig. S5 *M* vs *H* curve of **1**