

Supplementary Information

Crystal structure and thermodynamic properties of dinickel diphosphate dihydrate $\text{Ni}_2(\text{H}_2\text{O})_2[\text{P}_2\text{O}_7]$

Galina V. Kiriukhina,^{*a,b} Olga V. Yakubovich,^a Larisa V. Shvanskaya,^{a,c} Yevgeniy A. Ovchenkov,^a Anatoly S. Volkov,^{a,b} Olga V. Dimitrova,^a Sergey V. Simonov^d and Alexander N. Vasiliev^{a,e}

^aLomonosov Moscow State University, Moscow 119991, Russia.

^bInstitute of Experimental Mineralogy RAS, Chernogolovka, 142432, Russia.

^cNational University of Science and Technology "MISIS", Moscow 119049, Russia.

^dInstitute of Solid State Physics, RAS, Chernogolovka 142432, Russia.

^eNational Research South Ural State University, Chelyabinsk 454080, Russia.

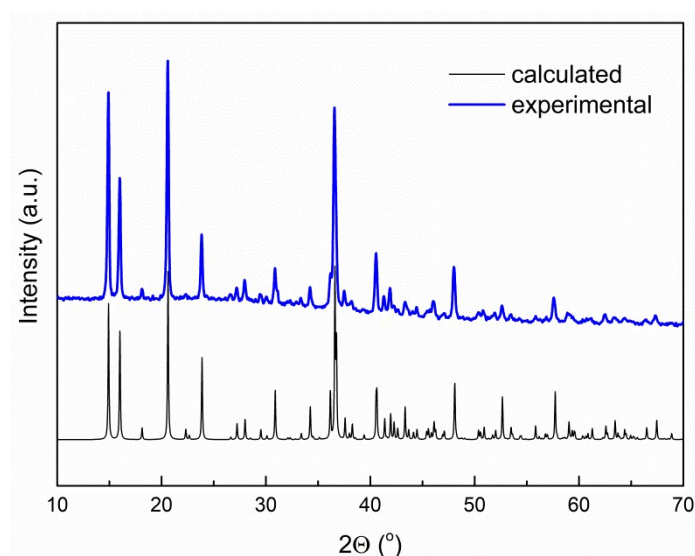


Figure S1. Experimental and calculated powder XRD pattern of the titled compound.

The powder XRD analysis was performed by an ADP-2 diffractometer using $\text{CoK}\alpha$ radiation, $\lambda=1.7903 \text{ \AA}$. The experimental powder pattern is in agreement with the simulated one on the basis of single crystal structural data. No impurity peaks are observed.

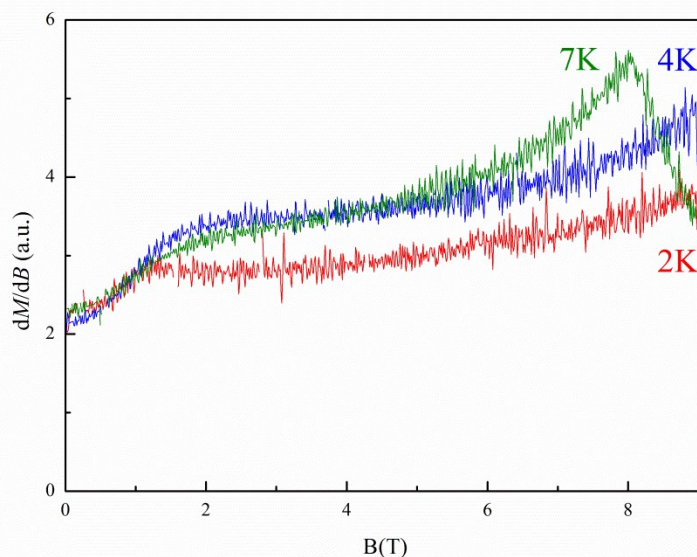


Figure S2. Field dependences of dM/dB in $\text{Ni}_2(\text{H}_2\text{O})_2[\text{P}_2\text{O}_7]$ at various temperatures.

Table S1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.26753(3)	0.11435(2)	0.58497(3)	0.00381(6)
Ni2	0.04756(3)	0.24996(2)	0.85186(3)	0.00391(6)
P1	0.26032(7)	0.41674(3)	0.14949(6)	0.00345(9)
P2	0.06421(7)	0.31199(3)	0.43021(6)	0.00348(9)
O1	0.16688(18)	0.40781(8)	0.34815(15)	0.0044(2)
O2	-	0.29078(9)	0.30787(16)	0.0053(2)
	0.14062(18)			
O3	0.22883(18)	0.23073(9)	0.40779(16)	0.0055(2)
O4	0.19582(18)	0.02255(8)	0.37492(16)	0.0057(2)
O5	0.08545(18)	0.37282(8)	0.01641(16)	0.0051(2)
O6	0.02929(19)	0.33884(8)	0.62560(15)	0.0057(2)
O7	0.46539(18)	0.35650(9)	0.16058(16)	0.0052(2)
O8	0.2576(2)	0.00567(9)	0.77691(17)	0.0084(2)
O9	0.0632(2)	0.14883(10)	1.06083(18)	0.0090(2)
H1	0.343(5)	-0.040(2)	0.802(4)	0.037(8)*
H2	0.137(5)	-0.020(2)	0.772(4)	0.048(9)*
H3	0.084(6)	0.170(3)	1.166(5)	0.070(12)*
H4	0.160(7)	0.111(3)	1.039(6)	0.094(16)*