Supporting Information

Crystal Structure and Magnetic Properties of $Pb_2Ni(PO_4)_2$

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Pb_2Ni(PO_4)_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pb(1)	2501(1)	4923(1)	8234(1)	11(1)
Pb(2)	-2633(1)	7640(1)	3183(1)	10(1)
Ni(1)	-7831(3)	6354(1)	4791(2)	7(1)
P(1)	-7402(5)	6647(2)	941(3)	7(1)
P(2)	-2430(5)	9256(1)	773(3)	5(1)
O(1)	-4922(13)	6529(5)	-4(8)	15(2)
O(2)	-6695(14)	6818(4)	2685(9)	15(2)
O(3)	-8983(14)	7409(4)	316(9)	12(1)
O(4)	-8995(13)	5806(4)	733(8)	11(1)
O(5)	-3196(13)	10182(4)	1047(8)	8(1)
O(6)	-1486(14)	9041(4)	-935(8)	9(1)
O(7)	-126(13)	9027(4)	1849(8)	8(1)
O(8)	-4614(13)	8618(4)	1169(8)	9(1)

Table S2. Selected bond lengths [Å] and angles (deg.) for $Pb_2Ni(PO_4)_2$

Pb(1)-O(4)#1	2.338(7)	Pb(1)-O(6)#2	2.431(7)
Pb(1)-O(7)#3	2.435(7)	Pb(1)-O(4)#4	2.634(7)
Pb(1)-O(1)	2.984(7)	Pb(1)-O(5)	2.934(7)
Pb(2)-O(1)#3	2.336(7)	Pb(2)-O(8)	2.504(7)
Pb(2)-O(2)	2.529(8)	Pb(2)-O(3)#5	2.638(8)
Pb(2)-O(6)	2.771(7)	Pb(2)-O(7)	2.762(8)
Ni(1)-O(2)	2.009(7)	Ni(1)-O(5)#6	2.019(6)
Ni(1)-O(3)#3	2.056(7)	Ni(1)-O(8)#3	2.059(7)
Ni(1)-O(6)#7	2.116(7)	Ni(1)-O(7)#7	2.199(7)
P(1)-O(3)	1.538(7)	P(1)-O(2)	1.540(8)
P(1)-O(1)	1.545(7)	P(1)-O(4)	1.559(7)
P(2)-O(5)	1.507(6)	P(2)-O(8)	1.555(7)
P(2)-O(7)	1.559(8)	P(2)-O(6)	1.561(7)
O(2)-Ni(1)-O(5)#6	86.0(3)	O(2)-Ni(1)-O(3)#3	86.9(3)
O(5)#6-Ni(1)-O(3)#3	171.9(3)	O(2)-Ni(1)-O(8)#3	104.2(3)
O(5)#6-Ni(1)-O(8)#3	89.7(3)	O(3)#3-Ni(1)-O(8)#3	95.9(3)
O(2)-Ni(1)-O(6)#7	96.9(3)	O(5)#6-Ni(1)-O(6)#7	83.4(3)
O(3)#3-Ni(1)-O(6)#7	93.5(3)	O(8)#3-Ni(1)-O(6)#7	157.3(3)
O(2)-Ni(1)-O(7)#7	163.6(3)	O(5)#6-Ni(1)-O(7)#7	100.7(2)
O(3)#3-Ni(1)-O(7)#7	85.1(3)	O(8)#3-Ni(1)-O(7)#7	90.9(3)
O(6)#7-Ni(1)-O(7)#7	69.4(3)		
O(3)-P(1)-O(2)	109.1(4)	O(3)-P(1)-O(1)	111.9(4)
O(2)-P(1)-O(1)	107.9(4)	O(3)-P(1)-O(4)	107.9(4)
O(2)-P(1)-O(4)	112.4(4)	O(1)-P(1)-O(4)	107.6(4)
O(5)-P(2)-O(8)	111.8(4)	O(5)-P(2)-O(7)	109.7(4)
O(8)-P(2)-O(7)	108.1(4)	O(5)-P(2)-O(6)	115.5(4)
O(8)-P(2)-O(6)	107.5(4)	O(7)-P(2)-O(6)	103.9(4)

Symmetry transformations used to generate equivalent atoms:

#1-x-1,-y+1,-z+1 #2 -x,y-1/2,-z+1/2 #3 x,-y+3/2,z+1/2 #4 x+1,y,z+1

#5 x+1,-y+3/2,z+1/2 #6 -x-1,y-1/2,-z+1/2 #7 x-1,-y+3/2,z+1/2

#8 x+1,-y+3/2,z-1/2 #9 x,-y+3/2,z-1/2 #10 x-1,-y+3/2,z-1/2 #11 x-1,y,z-1

#12 -x-1,y+1/2,-z+1/2 #13 -x,y+1/2,-z+1/2

Table S3. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Pb_2Ni(PO_4)_2$. The anisotropic displacement factor exponent takes the form:$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pb(1)	17(1)	7(1)	7(1)	0(1)	1(1)	-1(1)
Pb(2)	19(1)	6(1)	7(1)	2(1)	2(1)	1(1)
Ni(1)	14(1)	3(1)	5(1)	1(1)	1(1)	0(1)
P(1)	14(1)	3(1)	4(1)	1(1)	3(1)	-1(1)
P(2)	10(1)	3(1)	3(1)	1(1)	2(1)	0(1)
O(1)	15(2)	14(2)	15(2)	0(1)	1(1)	0(1)
O(2)	16(2)	15(2)	15(2)	0(1)	0(1)	-1(1)
O(3)	13(2)	12(2)	13(2)	1(1)	0(1)	0(1)
O(4)	11(2)	11(2)	11(2)	0(1)	0(1)	0(1)
O(5)	8(2)	7(2)	8(2)	-1(1)	0(1)	0(1)
O(6)	10(2)	9(2)	8(2)	0(1)	0(1)	0(1)
O(7)	9(2)	8(2)	8(2)	0(1)	0(1)	0(1)
O(8)	9(2)	8(2)	9(2)	1(1)	0(1)	-1(1)