Ionothermal Synthesis, Crystal Structure, and Magnetic Study of Co_2PO_4OH Isostructural with Caminite

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Table S1. Crystal data and structure refinement for $Co_2(PO_4)OH$

Identification code	1
Empirical formula	$Co_2(PO_4)OH$
Formula weight (g / mol)	919.35
Temperature (K)	293(2)
Wavelength	0.71073 Å
Crystal system, space group	tetragonal, $I4_1/amd$
Unit cell dimensions a=b (Å)	5.2713(7)
c (Å)	12.907(3)
Volume ($Å^3$)	358.64(11)
Z, calculated density (mg/m^3)	4, 4.257
Absorption coefficient (mm^{-1})	9.584
F(000)	440
Theta range for data collection	4.18 to 27.43 °.
Limiting indices	$-6 \leq h \leq 7$, $-6 \leq k \leq 6$, $-16 \leq l \leq 16$
Reflections collected / unique	1535 / 130 [R(int) = 0.0647]
Completeness to	θ = 27.43 100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	130 / 0 / 15
Goodness-of-fit on F^2	1.220
Final R indices [I>2σ(I)]	R1 = 0.0870, wR2 = 0.2490

R indices (all data)	R1 = 0.0896, wR2 = 0.2536
Largest diff. peak and hole	3.124 and -1.317 e.Å^{-3}

Table S2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 ×10^3) for $Co_2(PO_4)OH$ (**1**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	-7500	-2500	2500	32(2)
P(1)	-5000	-7500	1250	9(2)
O(1)	-5000	-5172(16)	1931(8)	16(2)
O(1H)	5000	-2500	1250	10(3)

Table S3. Bond lengths [Å] and angles [°] for $Co_2(PO_4)OH$ (**1**) .

Co(1)-O(1)#1	2.064(6)	Co(1)-Co(1)#4	2.6356(4)
Co(1)-O(1)#2	2.064(6)	Co(1)-Co(1)#2	2.6356(4)
Co(1)-O(1)#3	2.064(6)	P(1)-O(1)	1.510(8)
Co(1)-O(1)	2.064(6)	P(1)-O(1)#5	1.510(8)
Co(1)-O(1H)#3	2.0832(3)	P(1)-O(1)#6	1.510(8)
Co(1)-O(1H)	2.0832(3))	P(1)-O(1)#7	1.510(8)

O(1)#1-Co(1)-O(1)#2	180.0(5)	O(1)#2-Co(1)-Co(1)#2	50.32(15)
O(1)#1-Co(1)-O(1)#3	86.1(4)	O(1)#3-Co(1)-Co(1)#2	129.68(15)
O(1)#2-Co(1)-O(1)#3	93.9(4)	O(1)-Co(1)-Co(1)#2	50.32(15)
O(1)#1-Co(1)-O(1)	93.9(4)	O(1H)#3-Co(1)-Co(1)#2	50.758(7)
O(1)#2-Co(1)-O(1)	86.1(4)	O(1H)-Co(1)-Co(1)#2	129.242(8)
O(1)#3-Co(1)-O(1)	180.0(5)	Co(1)#4-Co(1)-Co(1)#2	180.0
O(1)#1-Co(1)-O(1H)#3	97.4(2)	O(1)-P(1)-O(1)#5	109.8(4)
O(1)#2-Co(1)-O(1H)#3	82.6(2)	O(1)-P(1)-O(1)#6	109.8(4)
O(1)#3-Co(1)-O(1H)#3	97.4(2)	O(1)#5-P(1)-O(1)#6	108.7(8)
O(1)-Co(1)-O(1H)#3	82.6(2)	O(1)-P(1)-O(1)#7	108.7(8)
O(1)#1-Co(1)-O(1H)	82.6(2)	O(1)#5-P(1)-O(1)#7	109.8(4)
O(1)#2-Co(1)-O(1H)	97.4(2)	O(1)#6-P(1)-O(1)#7	109.8(4)
O(1)#3-Co(1)-O(1H)	82.6(2)	P(1)-O(1)-Co(1)#2	139.63(19)
O(1)-Co(1)-O(1H)	97.4(2)	P(1)-O(1)-Co(1)	139.63(19)
O(1H)#3-Co(1)-O(1H)	180.0	Co(1)#2-O(1)-Co(1)	79.4(3)
O(1)#1-Co(1)-Co(1)#4	50.32(15)	Co(1)#8-O(1H)-Co(1)	126.857(9)
O(1)#2-Co(1)-Co(1)#4	129.68(15)	Co(1)#8-O(1H)-Co(1)#9	78.485(15)
O(1)#3-Co(1)-Co(1)#4	50.32(15)	Co(1)-O(1H)-Co(1)#9	126.857(9)
O(1)-Co(1)-Co(1)#4	129.68(15)	Co(1)#8-O(1H)-Co(1)#4	126.857(9)
O(1H)#3-Co(1)-Co(1)#4	129.242(7)	Co(1)-O(1H)-Co(1)#4	
O(1H)-Co(1)-Co(1)#4	50.758(8)	Co(1)#9-O(1H)-Co(1)#4	
O(1)#1-Co(1)-Co(1)#2	129.68(15)		

Symmetry transformations used to generate equivalent atoms:

#1 -y+3/4,x+3/4,-z+1/4 #2 -x+0,-y+3/2,z+0

#3 y-3/4,-x+3/4,-z+1/4 #4 -x+1,-y+3/2,z+0

#5 x,y-1/2,-z #6 -x+1,-y+1,-z #7 -x+1,-y+1/2,z+0

#8 -y+5/4,x-1/4,z+1/4 #9 y-1/4,-x+3/4,z+1/4

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Co_2(PO_4)OH$ (**1**).

The anisotropic displacement factor exponent takes the form:

$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Co(1)	54(2)	24(2)	18(2)	0	-1(1)	0
P(1)	11(2)	11(2)	6(3)	0	0	0
O(1)	25(5)	11(4)	13(5)	-11(3)	0	0
O(1H)	13(5)	13(5)	3(6)	0	0	0

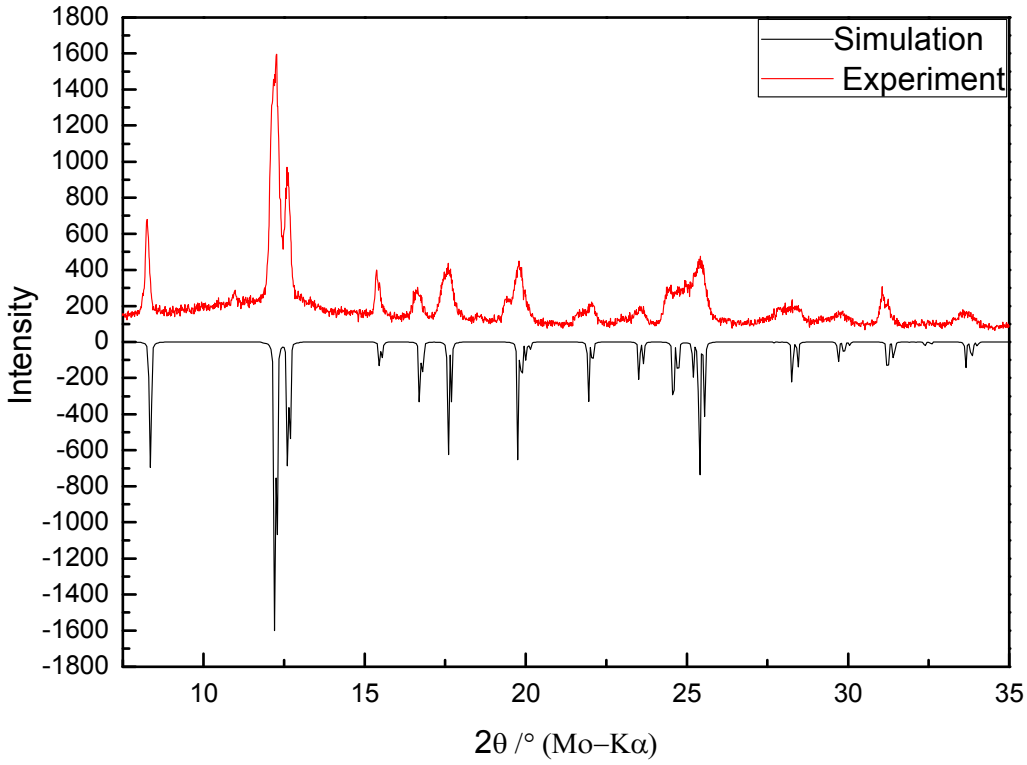

Figure S1. Experimental and simulated X-ray powder diffraction pattern of $Co_2(PO_4)OH$ (**1**).

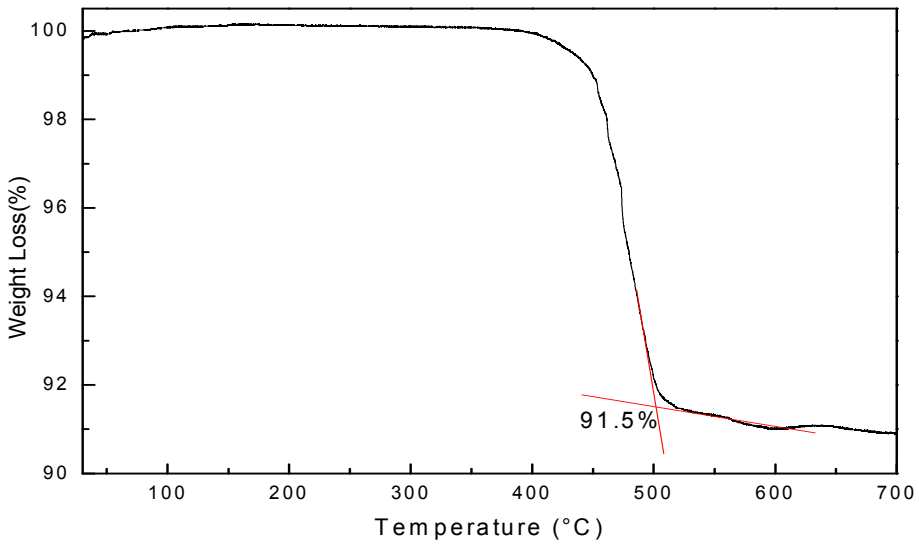

Figure S2. TG curve of $Co_2(PO_4)OH$ (**1**).

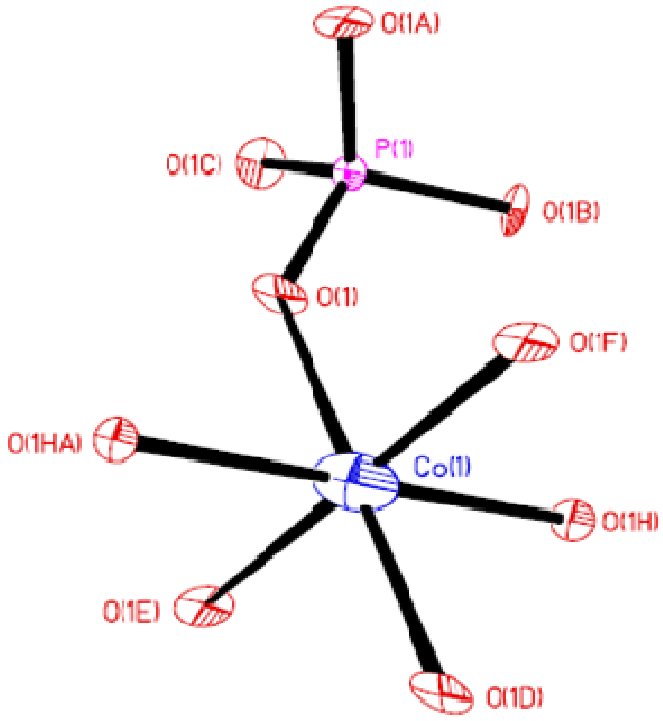

Figure S3. Thermal ellipsoid plot (50% probability) and atomic labeling scheme for $Co_2(PO_4)OH$ (**1**).