Supporting Materials

Synthesis of New Framework Cobalt Aluminophosphate by Opening Cobalt Methylphosphonate Layered Material

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Table S1. Positional parameters of $Co_{1.16}Al_2P_4O_{20}H_{12}$ in the space group $P2_1/n$ with a=8.402(4)Å, b=16.569(7)Å, c=5.11(1)Å and β=90.6°.

Atom	Wyckoff position	Occu-pancy	X	y	z	u_{eq} (Å²)
Co1	2d	1	0.5	0	0	0.0292(3)
P4	4e	1	0.80996(14)	-0.08670(6)	-0.2388(3)	0.0156(3)
Al1	4e	1	0.63583(15)	0.29195(7)	0.2465(3)	0.0132(3)
P2	4e	1	0.48742(13)	-0.19170(6)	0.2474(2)	0.0132(3)
Co2	2d	0.161(4)	0.5	0	-0.5	0.0107(15)
O1	4e	1	0.5124(4)	-0.09836(16)	0.2747(6)	0.0211(9)
O2	4e	1	0.6905(5)	0.05492(14)	0.2081(7)	0.0357(13)
O3	4e	1	0.9261(6)	-0.0112(2)	-0.2600(9)	0.0419(14)
O4	4e	1	0.4066(4)	-0.20174(16)	-0.0198(6)	0.0164(9)
O5	4e	1	0.3836(4)	-0.21853(16)	0.4712(6)	0.0151(9)
O6	4e	1	0.6403(5)	-0.0560(2)	-0.2723(7)	0.0313(11)
O7	4e	1	0.8533(4)	-0.14201(18)	-0.4570(6)	0.0200(10)
O8	4e	1	0.6472(4)	-0.23489(17)	0.2624(7)	0.0169(8)
O9	4e	1	0.0897(3)	0.81494(16)	0.2375(7)	0.0226(10)
O10	4e	1	0.8342(4)	-0.12060(18)	0.0310(6)	0.0207(10)
H1-O9	4e	1	0.1481	0.7871	0.146	0.027178
H2-O9	4e	1	0.1268	0.8525	0.3223	0.027178
H1-O2	4e	1	0.7779	0.033	0.2131	0.04282
H2-O2	4e	1	0.6766	0.0981	0.2833	0.04282
H1-O1	4e	1	0.5255	-0.0495	0.289	0.025354
H1-O3	4e	1	0.9859	0.0277	-0.2708	0.050317

Table S2. Details of the single crystal XRD data collection

Chemical formula	$Co_{1.16}\ Al_2\ P_4\ O_{20}\ H_{12}$
Molecularweight ($g.mol^{-1}$)	578.36
Space group	$P2_1/n$
a (Å)	8.402(4)
b (Å)	16.569(7)
*c (*Å)	5.11(1)
α (°)	90
β(°)	90.6(2)
γ (°)	90
Cell volume ($Å^3$)	711.2(16)
Z	2
Density ($g.cm^{-3}$)	*2.7009*
μ (mm^{-1})	*2.08*
Data collection temperature (K)	*293*
wavelength (Å)	0.71069
scan strategy / Dx (mm)	*ω/φ scan / 35*
Θmax	32.89
Reflections index limit	$-12 \leq h \leq 11$ $-24 \leq h \leq 24$ $-7 < h < 7$
unique reflections with I≥3*σ(*I)	1721
Absorption correction	multi-scan / SADABS
Internal R value after correction (%)	6.3
number of refinement parameters parameters	132
Number of restraints	8
ρmin/ *ρmax*(*e*/ $Å^3$)	-1.18/0.86
F(000)	579
Reliability factors	0.0581

Table S3. ADP harmonic parameters.

atoms	u_{11}(Å^2)	u_{22}(Å^2)	u_{33}(Å^2)	u_{12}(Å^2)	u_{13}(Å^2)	u_{23}(Å^2)
Co1	0.0221(6)	0.0196(4)	0.0457(7)	0.0053(5)	0.0109(7)	0.0087(4)
P4	0.0164(6)	0.0135(5)	0.0167(5)	0.0000(4)	0.0037(7)	0.0005(5)
Al1	0.0108(6)	0.0150(6)	0.0137(5)	0.0000(5)	0.0031(8)	0.0007(6)
P2	0.0107(5)	0.0154(5)	0.0134(4)	-0.0018(4)	0.0028(7)	-0.0013(5)
Co2	0.012(3)	0.006(2)	0.014(3)	0.002(2)	-0.002(3)	-0.0059(18)
O1	0.0215(17)	0.0118(13)	0.0301(16)	-0.0051(13)	0.0025(19)	-0.0047(13)
O2	0.035(2)	0.0193(17)	0.053(3)	0.0075(17)	-0.006(2)	-0.0037(19)
O3	0.050(3)	0.0301(19)	0.046(2)	-0.0254(19)	0.000(3)	-0.001(2)
O4	0.0179(19)	0.0168(14)	0.0144(15)	-0.0014(14)	-0.0001(14)	0.0016(12)
O5	0.0131(18)	0.0171(14)	0.0152(15)	0.0006(13)	0.0037(13)	0.0013(12)
O6	0.0230(19)	0.0336(18)	0.038(2)	0.0136(16)	0.001(2)	-0.001(2)
O7	0.021(2)	0.0194(15)	0.0192(15)	0.0033(15)	-0.0008(15)	-0.0023(13)
O8	0.0115(15)	0.0159(13)	0.0233(14)	-0.0010(12)	0.0019(18)	0.0015(14)
O9	0.0156(16)	0.0277(17)	0.0246(17)	-0.0001(14)	-0.0021(18)	-0.0100(17)
O10	0.022(2)	0.0208(15)	0.0194(16)	0.0048(15)	0.0009(17)	-0.0007(13)

Table S4: Interatomic distances. Symmetry codes: (i) -x+1,-y,-z ; (ii) -x+1,-y,-z+1 ; (iii) -x+3/2,y+1/2,-z-1/2 ; (iv) -x+3/2,y+1/2,-z+1/2 ; (v) -x+1/2,y-1/2,-z+1/2 ; (vi) x,y,z-1 ; (vii) -x+1,-y,-z-1.

	d (Å)		d (Å)		d (Å)
Co1-O1	2.153(5)	Co2-O1^{vi}	1.998(4)	Al1-O4^{i}	1.924(4)
Co1-O1^{i}	2.153(5)	Co2-O1^{i}	1.998(4)	Al1-O5^{ii}	1.894(6)
Co1-O2	2.126(5)	Co2-O2^{vi}	2.370(6)	Al1-O7^{iii}	1.842(6)
Co1-O2^{i}	2.126(5)	Co2-O2i	2.370(6)	Al1-O8^{iv}	1.877(4)
Co1-O6	2.046(6)	Co2-O6	1.898(5)	Al1-O9^{v}	1.934(3)
Co1-O6^{i}	2.046(6)	Co2-O6^{vii}	1.898(5)	Al1-O10^{iv}	1.859(5)
P4-O3	1.590(4)	P2-O1	1.567(3)		
P4-O6	1.523(4)	P2-O4	1.534(6)		
P4-O7	1.488(5)	P2-O5	1.505(5)		
P4-O10	1.503(7)	P2-O8	1.523(3)		

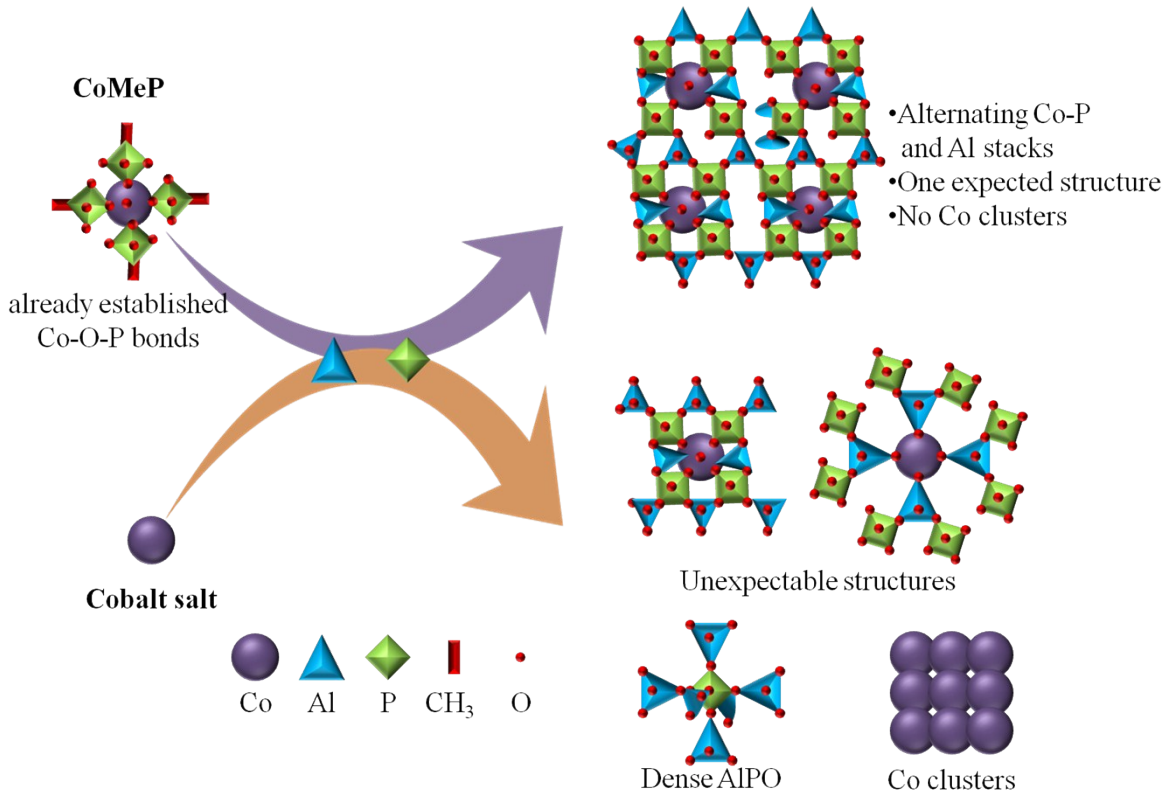

Figure S1. Simplified presentation of Co-AlPO formation starting from CoMeP versus cobalt salt.

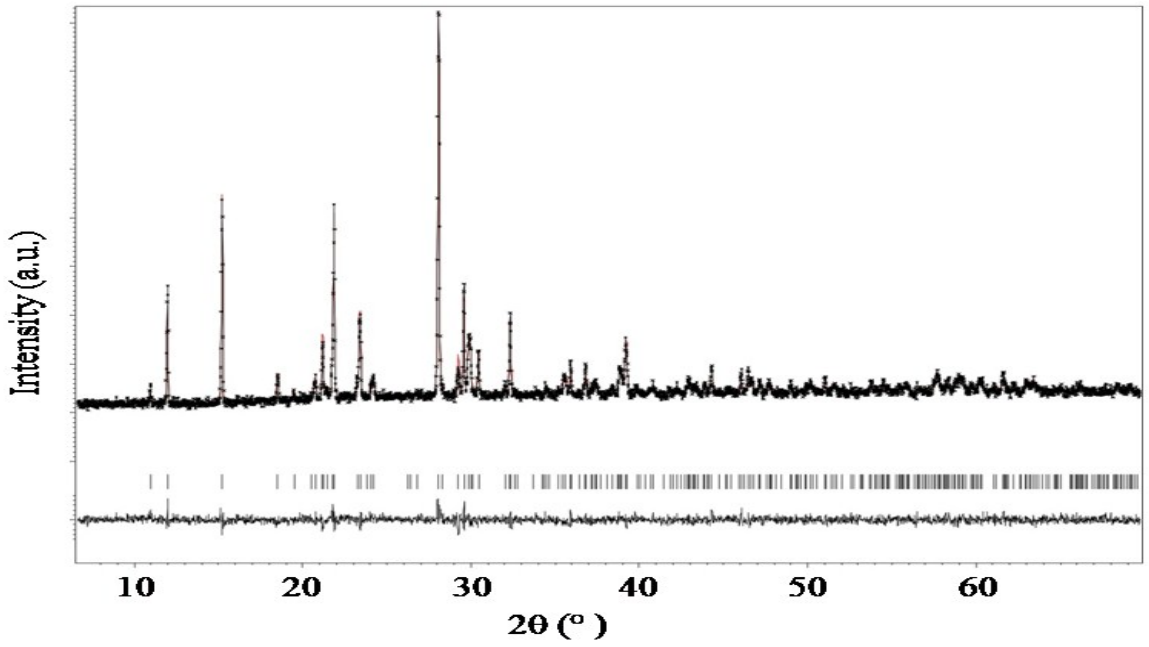

Figure S2. Rietveld refinement of the powder XRD pattern (Co-AlPO-4h) performed based on the structure obtained by single crystal XRD. The good matching confirms that the proposed structure of Co-AlPO is representative of the whole powder, which also appears free from secondary phase.