

Supporting Information

Synthesis and magnetic properties of two isostructural fluorophosphates BaMPO₄F (M = Cu, Co) with a tunnel structure

Chaoqun Qiu^{a,b}, Zhangzhen He^{a,*}, Meiyan Cui^{a,b}, and Sihuai Chen^a

^aState Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China.

^bUniversity of Chinese Academy of Sciences, Beijing, 100039, China.

*E-mail: hcz1988@hotmail.com; hezz@fjirsm.ac.cn

Figure S1. Experimental and simulated powder X-ray diffraction patterns of BaMPO₄F (M = Cu and Co).

Figure S2. View of the oxygen coordination environments for P, Cu, and Ba.

Figure S3. Diamond drawing for the structure of BaCuPO₄F in its asymmetric unit.

Figure S4. The susceptibility measured with FC and ZFC regimes for BaCoPO₄F.

Table S1. The Wyckoff positions, atomic coordinates, and equivalent isotropic displacement parameters of BaCuPO₄F.

Table S2. Anisotropic displacement parameters of BaCuPO₄F.

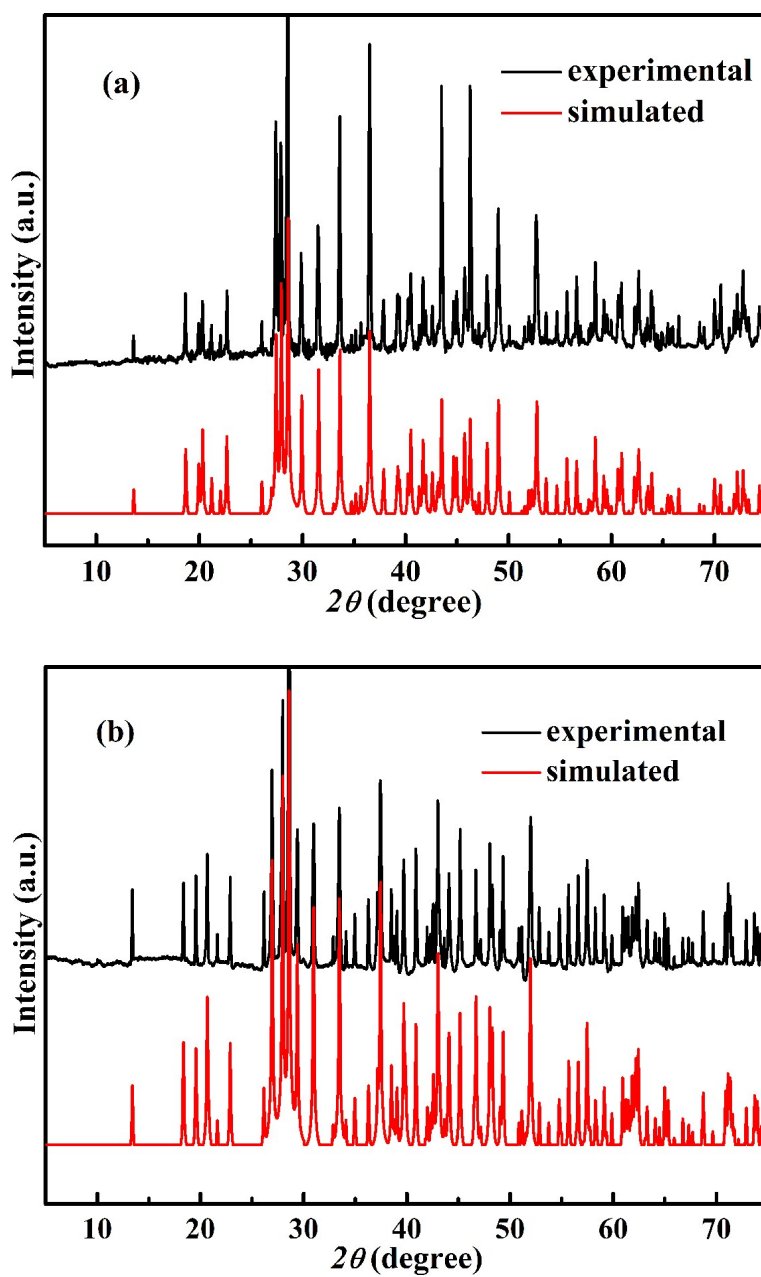


Figure S1. Experimental (Black line) and Simulated (Red line) powder X-ray diffraction patterns of BaCuPO_4F (a) and BaCoPO_4F (b).

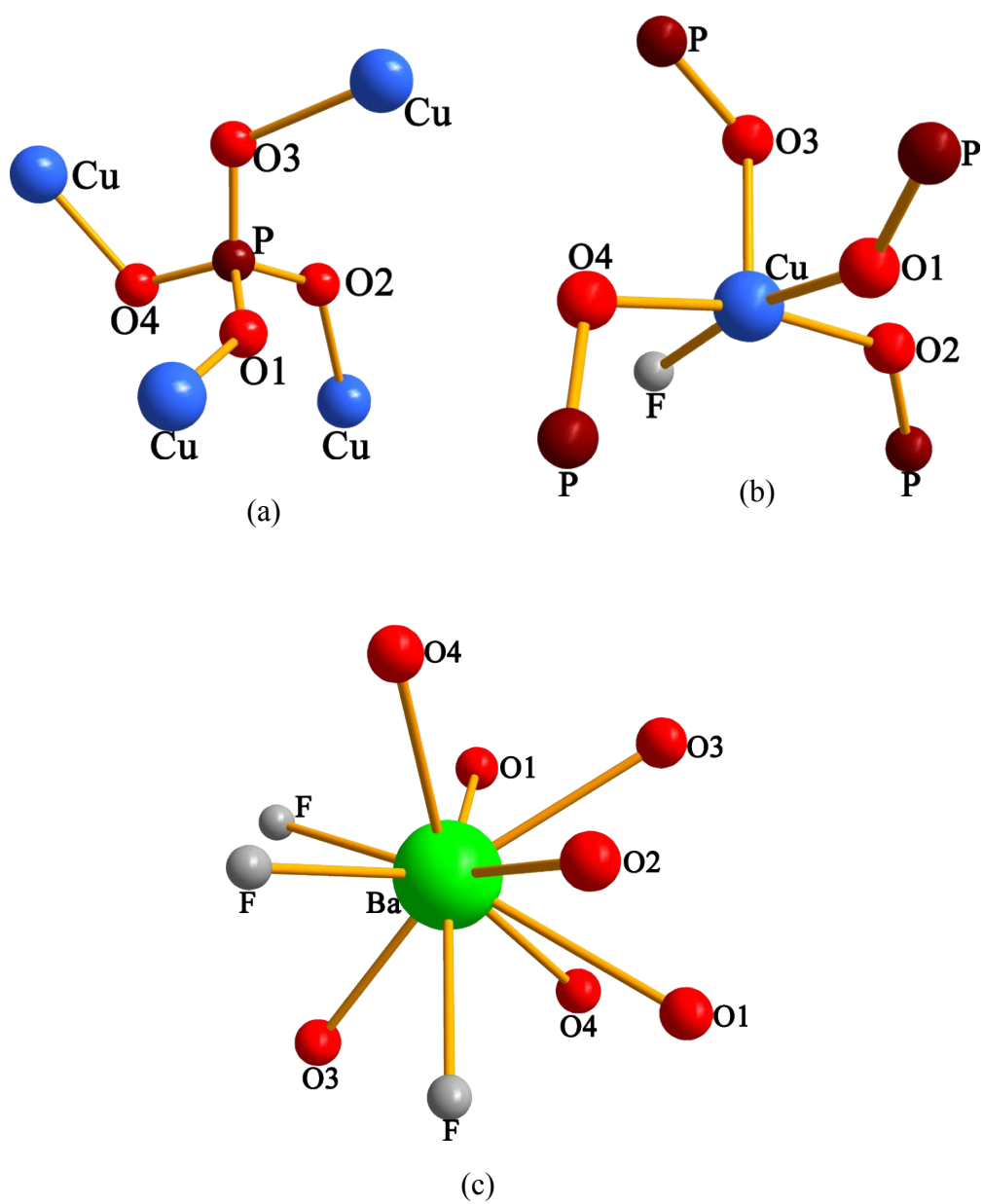


Figure S2. View of the oxygen coordination environments for (a) P, (b) Cu, and (c)

Ba.

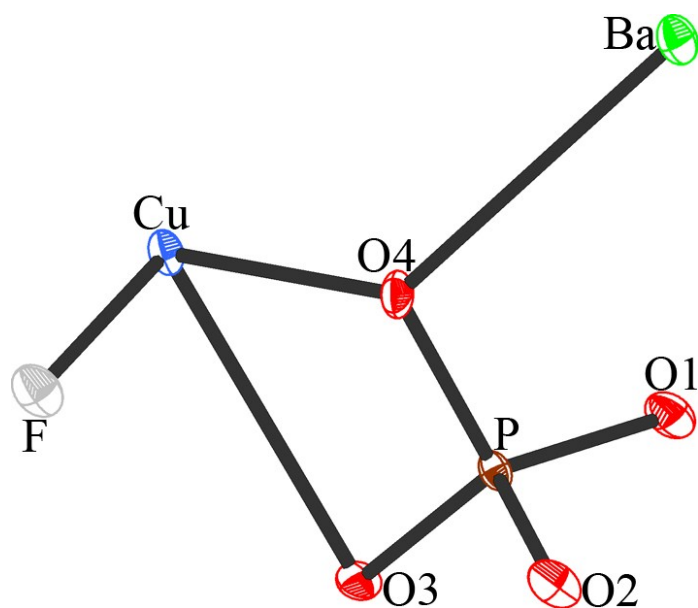


Figure S3. Diamond (50% probability ellipsoids) drawing for the structure of BaCuPO₄F in its asymmetric unit.

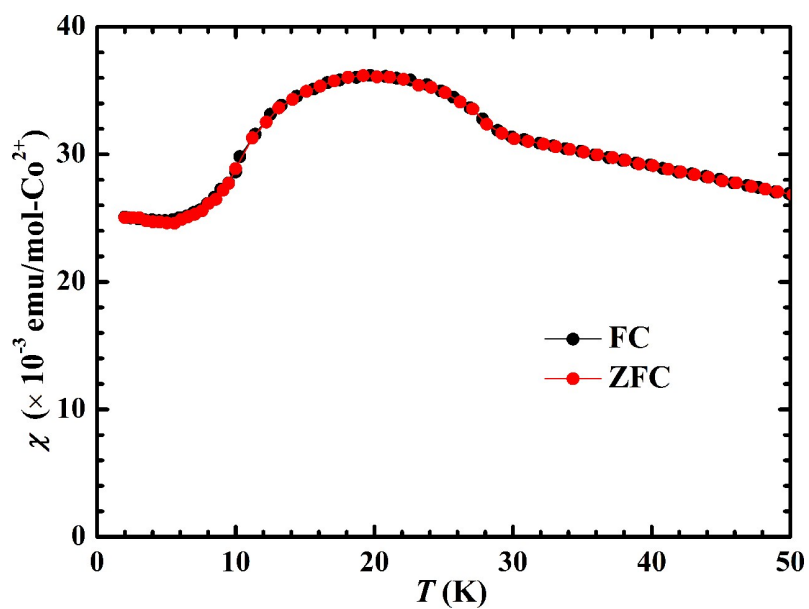


Figure S4. The susceptibility measured at 1000 Oe with FC and ZFC regimes for BaCoPO₄F

Table S1. The Wyckoff positions, atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) of BaCuPO₄F. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	Wyck.	Site	x	y	z	U(eq)
Ba	4a	1	-158(1)	7619(1)	8074(1)	11(1)
Cu	4a	1	-122(2)	5479(1)	4055(1)	8(1)
P	4a	1	4570(3)	5794(2)	5896(1)	7(1)
F	4a	1	168(7)	3329(3)	4239(3)	14(1)
O(1)	4a	1	5366(7)	7404(4)	6292(4)	12(1)
O(2)	4a	1	5828(8)	4727(4)	6983(3)	12(1)
O(3)	4a	1	5479(7)	5372(4)	4397(3)	10(1)
O(4)	4a	1	1440(7)	5627(4)	5991(3)	11(1)

Table S2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) of BaCuPO₄F. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

atom	U11	U22	U33	U23	U13	U12
Ba	14(1)	11(1)	8(1)	-1(1)	0(1)	0(1)
Cu	12(1)	7(1)	7(1)	0(1)	-1(1)	0(1)
P	9(1)	6(1)	5(1)	-1(1)	1(1)	-1(1)
F	20(2)	10(1)	11(1)	1(1)	-1(1)	4(1)
O(1)	16(2)	8(2)	13(2)	0(1)	0(1)	3(2)
O(2)	19(2)	11(2)	6(2)	3(1)	0(1)	6(2)
O(3)	9(2)	14(2)	6(1)	-1(1)	3(1)	2(2)
O(4)	10(2)	14(2)	7(1)	-4(1)	0(1)	-3(2)