SUPPORTING INFORMATION

Crystal structure and physical properties of shchurovskyite-related $K_2CaCu_6O_2(PO_4)_4$

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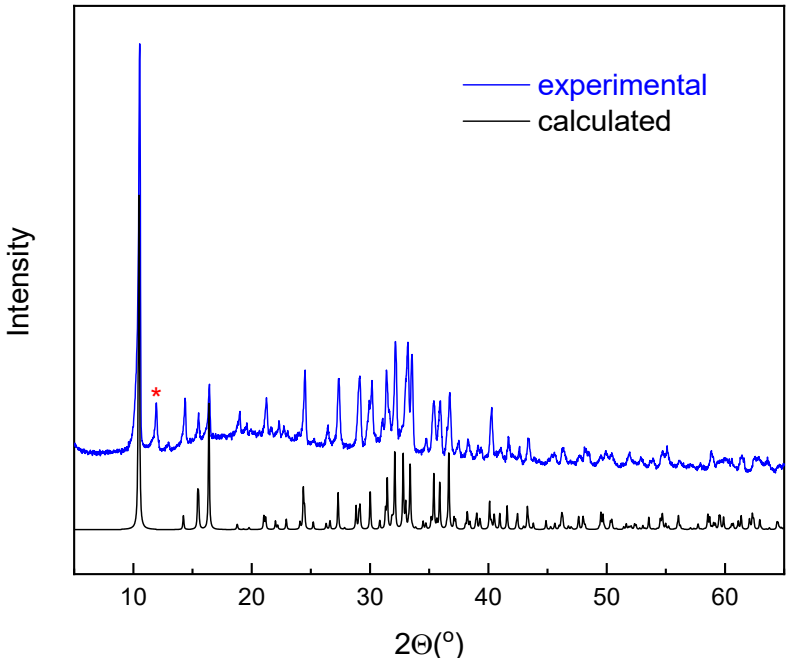

Fig. S1. Experimental and calculated X-Ray powder diffraction patterns for $K_2CaCu_6O_2(PO_4)_4$. The asterisk marks the impurity phase, identified as $Ca_3Cu_3(PO_4)_4$.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for $K_2(Ca_{0.876}Cu_{0.124})Cu_6O_2(PO_4)_4$*.

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5	0.88451(14)	0.75	0.0094(2)
Cu2	0.5	0.39424(14)	0.75	0.0126(2)
Cu3	0.46883(8)	0.67543(11)	0.57146(4)	0.01541(18)
Cu4	0.77548(8)	0.66215(11)	0.66320(4)	0.01356(18)
Cu5	1.0	0.1649(2)	0.75	0.0135(5)
Ca1	1.0	0.1649(2)	0.75	0.0135(5)
P1	0.35185(17)	0.8297(2)	0.39321(8)	0.0070(3)
P2	1.14463(17)	0.6898(2)	0.65766(8)	0.0102(3)
K1	0.219(3)	1.193(3)	0.5616(11)	0.0662(19)
K2	0.1440(12)	1.2064(7)	0.5413(4)	0.0662(19)

O1	0.5528(4)	0.6358(5)	0.67856(19)	0.0080(8)
O2	0.4657(4)	0.8575(5)	0.3245(2)	0.0118(8)
O3	0.3266(4)	1.0758(5)	0.4279(2)	0.0096(8)
O4	0.4414(4)	0.6701(5)	0.4565(2)	0.0108(8)
O5	0.1965(4)	0.7104(5)	0.3610(2)	0.0130(8)
O6	1.2467(4)	0.7344(6)	0.5878(2)	0.0186(9)
O7	1.1935(5)	0.8574(6)	0.7285(2)	0.0205(9)
O8	0.9719(5)	0.7531(6)	0.6251(2)	0.0217(10)
O9	1.1576(5)	0.4346(6)	0.6859(2)	0.0239(10)

*Refined occupancies for Cu5 and Ca1 are 0.124(8) and 0.876(8); for K1 and K2 are 0.22(2) and 0.79(2).

Table S2. Interatomic distances (Å^2) for $K_2(Ca_{0.876}Cu_{0.124})Cu_6O_2(PO_4)_4$.

Cu1 octahedron		Cu2 planar square		Cu3 5-vertex polyhedron		Cu4 5-vertex polyhedron	
Cu1-O1	1.925(3)×2	Cu2-O1	1.896(3)×2	Cu3-O1	1.894(3)	Cu4-O8	1.881(4)
-O2	1.960(3)×2	-O2	1.934(3)×2	-O6	1.927(4)	-O1	1.905(4)
-O7	2.652(3)×2	-O9	2.983(3)×2	-O4	1.931(3)	-O7	2.130(4)
				-O4	2.159(3)	-O5	2.164(3)
				-O3	2.213(3)	-O3	2.251(3)
						-O9	2.863(3)

Ca1 octahedron*		K1* 9-vertex polyhedron		K2* 8-vertex polyhedron		P1 tetrahedron		P2 tetrahedron	
Ca1-O9	2.336(4)×2	K1-O3	2.58(2)	K2-O3	2.644(5)	P1-O5	1.523(4)	P2-O9	1.522(3)
-O7	2.422(4)×2	-O9	2.59(2)	-O9	2.749(6)	-O3	1.531(3)	-O6	1.528(4)
-O5	2.489(4)×2	-O6	2.64(2)	-O6	2.894(7)	-O4	1.543(3)	-O8	1.544(4)
		-O4	2.98(3)	-O8	2.899(9)	-O2	1.564(3)	-O7	1.553(4)
		-O6	3.10(2)	-O6	3.189(6)				
		-O2	3.14(3)	-O8	3.311(5)				
		-O7	3.41(2)	-O5	3.429(8)				
		-O8	3.42(2)	-O4	3.534(8)				
		-O8	3.46(2)						

*Ca1 position is occupied by Ca and Cu for 0.876(8) and 0.124(8); refined occupancies for K1 and K2 are 0.215(19) and 0.785(19).

Table S3. Bond-valence data for the title phase.

Atom	K2	Ca1	Cu1	Cu2	Cu3	Cu4	P1	P2	∑
O1			$0.514^{\times 2\downarrow}$	$0.556^{\times 2\downarrow}$	0.559	0.543			2.17
O2			$0.468^{\times 2\downarrow}$	$0.502^{\times 2\downarrow}$			1.148		2.12
O3	0.259				0.236	0.213	1.255		1.96
O4	0.022				0.506, 0.273		1.215		2.02
O5	0.03	$0.244^{\times 2\downarrow}$				0.270	1.282		1.83
O6	0.127, 0.057				0.512			1.265	1.96
O7		$0.291^{\times 2\downarrow}$	$0.072^{\times 2\downarrow}$			0.296		1.182	1.84
O8	0.125					0.579		1.212	1.96

	0.041								
O9	0.188	0.369$^{\times 2\downarrow}$		0.029$^{\times 2\downarrow}$		0.041		1.286	1.91
∑	0.85	1.81	2.11	2.17	2.09	1.94	4.9	4.95	

The "large" distances for copper ions are taken into account. Signs $^{\times 2\downarrow}$ indicate doubling of the contribution according to symmetry. Atoms K1 with low occupancy are not considered.

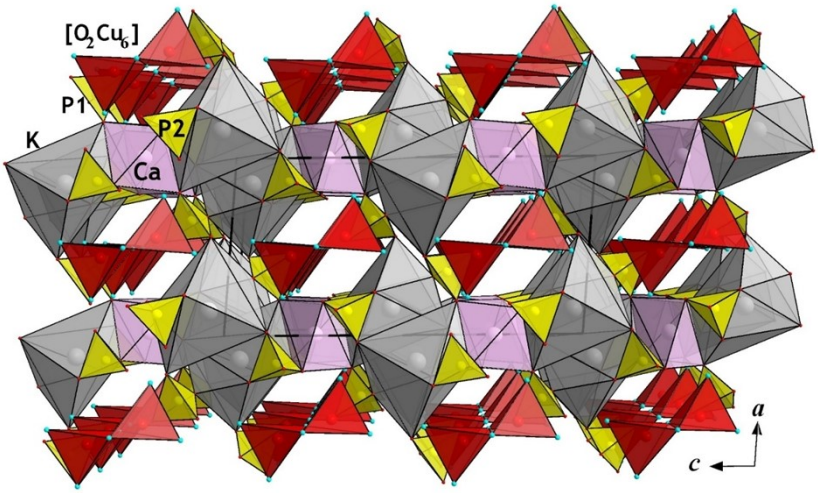

Figure S2. The *ac* projection of the $K_2CaCu_6O_2(PO_4)_4$ phase in the anion-centering approach.

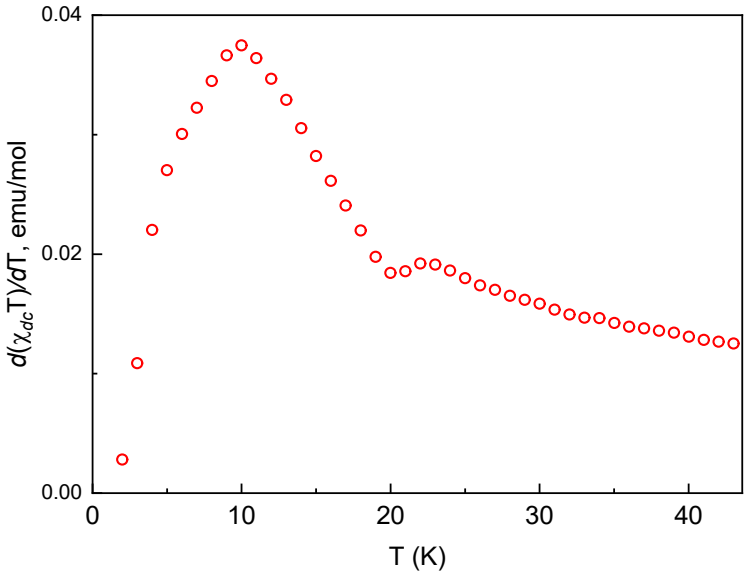

Figure S3. Temperature dependence of Fisher's specific heat, $d(\chi T)/dT$, in $K_2CaCu_6O_2(PO_4)_4$.