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Supporting information for article:

Rb2CaCu6(PO4)4O2, A NOVEL OXOPHOSPHATE WITH A SHCHUROVSKYITE-TYPE TOPOLOGY: SYNTHESIS, STRUCTURE, MAGNETIC PROPERTIES, AND CRYSTAL CHEMISTRY OF RUBIDIUM COPPER PHOSPHATES

Sergey M. Aksenov, Elena Yu. Borovikova, Vladimir S. Mironov, Natalia A. Yamnova, Anatoly S. Volkov, Dmitry A. Ksenofontov, Olga A. Gurbanova, Olga V. Dimitrova, Dina V. Deyneko, Elena A. Zvereva, Olga V. Maximova, Sergey V. Krivovichev, Peter C. Burns and Alexander N. Vasiliev

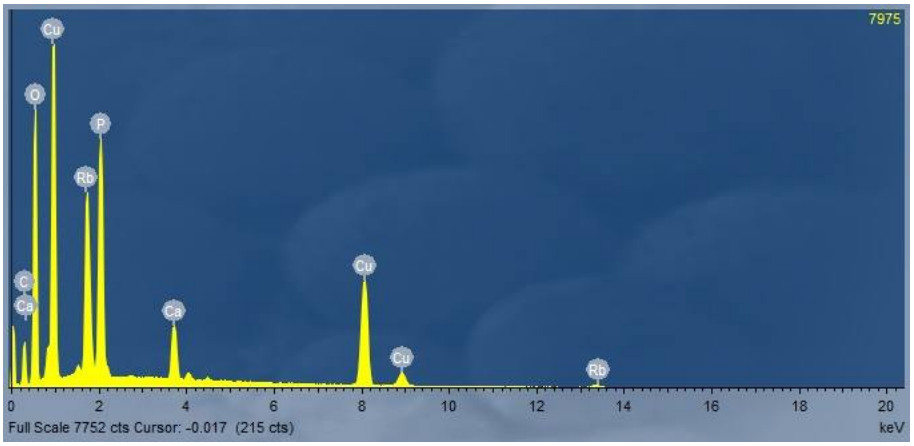


Figure S1 EDS spectrum of $Rb_2CaCu_6(PO_4)_4O_2$ compound.

Table S1 Chemical composition of $Rb_2CaCu_6(PO_4)_4O_2$ compound.

Element	Line	Weight %	Weight % sigma	Atomic %	Compound %	Formula	Standard
P	*K*-series	13.16	0.12	13.68	30.16	P_2O_5	GaP
Ca	*K*-series	3.84	0.07	3.09	5.38	CaO	Wollastonite
Cu	*K*-series	37.44	0.33	18.98	46.87	CuO	Cu
Rb	*K*-series	14.12	1.07	5.32	15.44	Rb_2O	$Rb_2Nb_4O_{11}$
O		29.28	0.4	58.93			
Total		97.85					

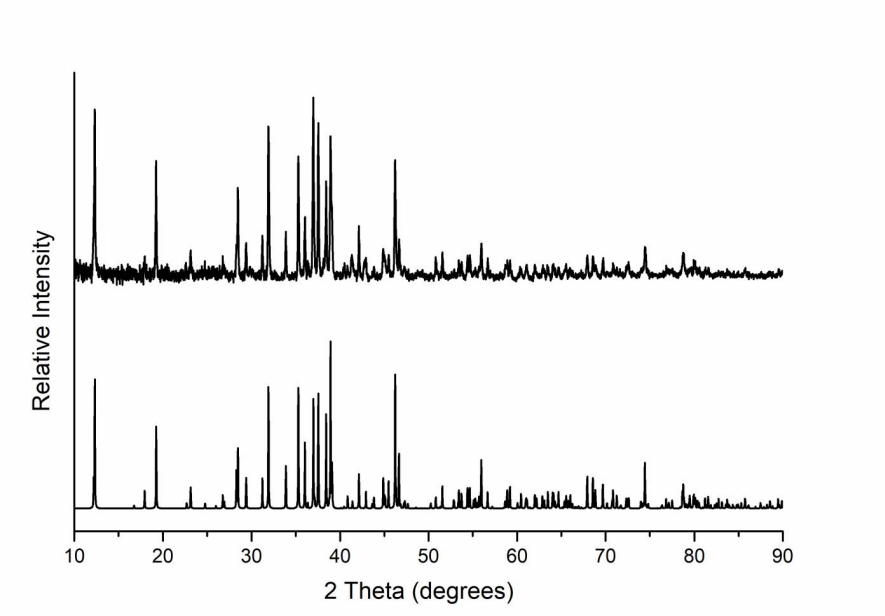


Figure S2. Experimental (top) and calculated (bottom) PXRD patterns of $Rb_2CaCu_6(PO_4)_4O_2$, λ = Co $K\alpha_1$.

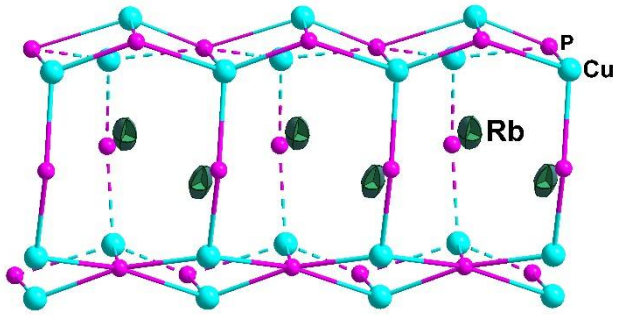
Table S2. Fractional atomic coordinates (*xyz*), site symmetry (*Q*), and equivalent atomic displacement parameters (U_{eq}) for $Rb_2Ca\{Cu_6O_2(PO_4)_4\}$.

Site	*x*	*y*	*z*	*Q*	U_{eq}
Rb	0.2901(1)	0.2062(2)	0.1575(2)	4	0.0344(2)
Cu1	0.3214(1)	-0.2582(1)	0.4727(1)	4	0.0096(1)
Cu2	0.5	0.4211(1)	0.5	2	0.0112(1)
Cu3	0.5	0.9130(1)	0.5	2	0.0092(1)
Cu4	0.0840(1)	0.1822(1)	0.2256(1)	4	0.0111(1)
Ca	0.5	0.1753(2)	0	2	0.0105(2)
P1	0.6448(1)	0.2009(2)	0.3518(1)	4	0.0069(2)
P2	0.4101(1)	-0.2931(2)	0.1483(1)	4	0.0089(2)
O1	0.3365(2)	-0.2696(6)	0.2451(3)	4	0.0136(6)
O2	0.5762(1)	0.1756(5)	0.4677(3)	4	0.0117(5)
O3	0.6138(2)	0.3236(5)	0.1953(4)	4	0.0135(6)
O4	0.0730(1)	0.1655(4)	0.4508(3)	4	0.0076(4)
O5	0.4764(2)	-0.1144(5)	0.2054(4)	4	0.0153(7)
O6	0.4428(2)	-0.5435(5)	0.1571(4)	4	0.0174(8)
O7	0.3822(2)	-0.2162(7)	-0.0248(4)	4	0.0188(8)
O8	0.7114(2)	0.3504(5)	0.4381(4)	4	0.0124(6)
O9	0.6746(2)	-0.0515(4)	0.3216(3)	4	0.0088(5)

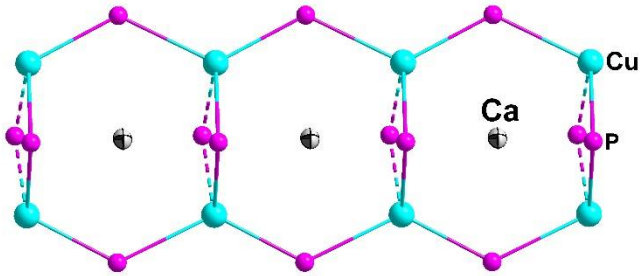
Note: U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Anisotropic atomic displacement parameters for $Rb_2Ca\{Cu_6O_2(PO_4)_4\}$.

Site	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb	0.0217(2)	0.0191(2)	0.0644(4)	0.0022(2)	0.0179(2)	-0.0025(2)
Cu1	0.0062(1)	0.0142(2)	0.0084(2)	0.0014(1)	0.0009(1)	-0.0011(1)
Cu2	0.0087(2)	0.0058(2)	0.0199(3)	0	0.0073(2)	0
Cu3	0.0080(2)	0.0061(2)	0.0142(3)	0	0.0041(2)	0
Cu4	0.0126(2)	0.0136(2)	0.0072(2)	0.0015(1)	0.0022(1)	0.0007(1)
Ca	0.0136(3)	0.0096(3)	0.0087(3)	0	0.0026(3)	0
P1	0.0062(2)	0.0064(3)	0.0083(3)	-0.0002(2)	0.0009(2)	-0.0002(2)
P2	0.0081(3)	0.0117(3)	0.0069(3)	0.0022(2)	0.0014(2)	0.0009(3)
O1	0.0107(8)	0.020(1)	0.010(1)	0.0020(9)	0.0038(8)	0.0004(9)
O2	0.0099(8)	0.0092(7)	0.017(1)	0.0005(7)	0.0069(8)	0.0003(9)
O3	0.017(1)	0.0123(9)	0.010(1)	0.0032(8)	-0.0020(9)	0.0007(8)
O4	0.0067(7)	0.0090(7)	0.0072(8)	-0.0009(6)	0.0006(6)	-0.0001(7)
O5	0.011(1)	0.016(1)	0.019(1)	-0.0035(8)	-0.001(1)	0.0010(9)
O6	0.018(1)	0.013(1)	0.021(2)	0.0064(9)	0.002(1)	-0.002(1)
O7	0.020(1)	0.029(2)	0.007(1)	0.011(1)	0.001(1)	0.001(1)
O8	0.0057(8)	0.0122(9)	0.019(1)	-0.0007(7)	0.0004(8)	-0.0050(9)
O9	0.0088(8)	0.0077(7)	0.010(1)	0.0018(6)	0.0022(8)	-0.0001(6)



(a)



(b)

Figure S3. Topology of the channels I (a) and II (b) in the crystal structure of $Rb_2Ca\{Cu_6O_2(PO_4)_4\}$.