

An open framework crystal structure and physical properties of $\text{RbCuAl}(\text{PO}_4)_2$

O. V. Yakubovich,^a G. V. Kiriukhina,^a O. V. Dimitrova,^a E. A. Zvereva,^a L. V. Shvanskaya,^{a,b} O.

S. Volkova^{a,b,c} and A. N. Vasiliev^{a,b,c}

^aM.V. Lomonosov Moscow State University, Moscow 119991, Russia

^bNational University of Science and Technology "MISIS", Moscow 119049, Russia

^cUral Federal University, Ekaterinburg 620002, Russia

Table S1. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2)

Atom	x/a	y/b	z/c	$U_{\text{eq}}/ U_{\text{iso}}$
Rb1	1.21380(8)	0.17410(3)	0.78709(4)	0.02163(13)
Cu1	1.23747(8)	0.45747(3)	0.95106(5)	0.01172(13)
P1	0.72625(17)	0.32801(6)	0.95098(10)	0.00910(19)
P2	1.28036(17)	0.48791(6)	0.66494(10)	0.00959(19)
Al1	0.7540(2)	0.37047(7)	0.61129(12)	0.0091(2)
O1	0.7703(5)	0.42219(17)	0.4248(3)	0.0153(5)
O2	1.4127(5)	0.40983(17)	0.5879(3)	0.0137(5)
O3	0.4349(5)	0.34030(16)	0.9698(3)	0.0131(5)
O4	0.7491(5)	0.31148(17)	0.7926(3)	0.0133(5)
O5	1.4524(5)	0.51013(17)	0.8134(3)	0.0117(5)
O6	1.0119(5)	0.44928(17)	0.6976(3)	0.0146(5)
O7	0.9046(5)	0.41436(16)	1.0148(3)	0.0110(5)
O8	0.8431(5)	0.25817(16)	0.5409(3)	0.0122(5)

Table S2. RbCuAl(PO₄)₂. Bond-valence data

Atom	Rb	Cu	Al	P1	P2	Σ
O1	0.086; 0.070		0.503		1.314	1.97
O2	0.097		0.681		1.248	2.03
O3	0.111; 0.046	0.487		1.262		1.91
O4	0.095; 0.050		0.520	1.279		1.94
O5	0.085	0.421; 0.100			1.248	1.85
O6	0.045	0.119	0.683		1.202	2.05
O7	0.106	0.411; 0.405		1.139		2.06
O8	0.124; 0.041		0.669	1.251		2.08
Σ	0.96	1.94	3.06	4.93	5.01	