Microstructures

Supplementary Material: $K_6Sn_4F_{12}I_2•0.5H_2O$: a Zero-Dimensional Alkali Metal Tin Mixed Halide Compound exhibiting color change due to crystal water loss

Supplementary Table 1. Crystal data and structure refinement for $K_6Sn_4F_{12}I_2•0.5H_2O$

	$K_6Sn_4F_{12}I_2•0.5H_2O$
Empirical formula	F48 H4 I8 K24 O2 Sn16
Formula weight	4800.99
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Cubic, Fd-3 m
Unit cell dimensions	a = 17.186(5) Å alpha = 90 deg.
	b = 17.186(5) Å beta = 90 deg.
	c = 17.186(5) Å gamma = 90 deg.
Volume	5076(4) $Å^3$
Z, calculated density	2, 3.141 mg/m^3
Absorption coefficient	7.381 mm^{-1}
F(000)	4264
Crystal size	0.120 mm × 0.100 mm × 0.080 mm
Theta range for data collection	2.052 to 28.456 deg.
Limiting indices	$-17 \leq h \leq 22$, $-22 \leq k \leq 22$, $-20 \leq l \leq 22$
Reflections collected/unique	7791/346 [R(int) = 0.0819]
Completeness to theta = 25.242	99.20%
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	346/1/18
Goodness-of-fit on F^2	1.092

Final R indices [I > 2sigma(I)]	R1 = 0.0491, wR2 = 0.1386
R indices (all data)	R1 = 0.0759, wR2 = 0.1770
Extinction coefficient	n/a
Largest diff. peak and hole	1.215 and -1.296 e. $Å^{-3}$

Supplementary Table 2. Atomic coordinates (× 10^{-4}) and equivalent isotropic displacement parameters ($Å^2$ × 10^{-3}) for $K_6Sn_4F_{12}I_2•0.5H_2O$

	x	y	z	U(eq)
Sn(1)	371(1)	2129(1)	371(1)	63(1)
F(1)	313(3)	3330(5)	313(3)	74(2)
I(1)	0	0	0	79(1)
O(1)	6250	1250	1250	26(7)
K(1)	1250	1250	4241(5)	118(2)

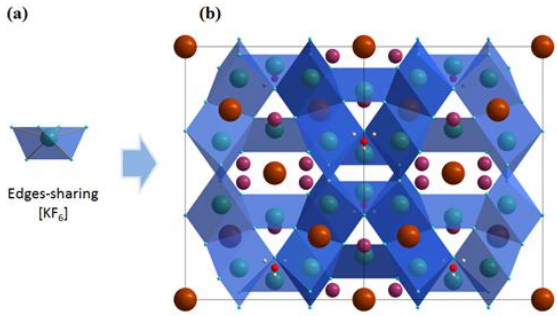
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Supplementary Table 3. Anisotropic displacement parameters ($Å^2$ × 10^{-3}) for $K_6Sn_4F_{12}I_2•0.5H_2O$

	U11	U22	U33	U23	U13	U12
Sn(1)	63(1)	63(1)	63(1)	3(1)	-3(1)	3(1)
F(1)	77(3)	67(5)	77(3)	1(3)	3(4)	1(3)
I(1)	79(1)	79(1)	79(1)	-9(1)	-9(1)	-9(1)
O(1)	26(7)	26(7)	26(7)	0	0	0
K(1)	104(3)	104(3)	146(6)	0	0	8(4)

Supplementary Table 4. Bond lengths [Å] and angles [deg.] for $K_6Sn_4F_{12}I_2•0.5H_2O$

Bond	Length	Angle	Degree
Sn(1)-F(1)	2.069(9)	F(1)-Sn(1)-F(1)#1	84.4(3)
Sn(1)-F(1)#1	2.069(9)	F(1)-Sn(1)-F(1)#2	84.4(3)
Sn(1)-F(1)#2	2.069(9)	F(1)#1-Sn(1)-F(1)#2	84.4(3)
O(1)-H(1W)	0.84(2)		



Supplementary Figure 1. The coordinating environment of K^+ cation and the crystal structure in the view of $[KF_6]$ polyhedra.