

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

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5 **Supplementary Table 1. Crystal data and structure refinement for**
6 **$K_6Sn_4F_{12}I_2 \cdot 0.5H_2O$**

	$K_6Sn_4F_{12}I_2 \cdot 0.5H_2O$
Empirical formula	F48 H4 I8 K24 O2 Sn16
Formula weight	4800.99
Temperature	293(2) K
Wavelength	0.71073 Å
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 ≤ h ≤ 22, -22 ≤ k ≤ 22, -20 ≤ l ≤ 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



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Final R indices [$I > 2\sigma(I)$]	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

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8 **Supplementary Table 2. Atomic coordinates ($\times 10^{-4}$) and equivalent isotropic**
9 **displacement parameters ($\text{Å}^2 \times 10^{-3}$) for $\text{K}_6\text{Sn}_4\text{F}_{12}\text{I}_2 \cdot 0.5\text{H}_2\text{O}$**

	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)

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

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12 **Supplementary Table 3. Anisotropic displacement parameters ($\text{Å}^2 \times 10^{-3}$) for**
13 **$\text{K}_6\text{Sn}_4\text{F}_{12}\text{I}_2 \cdot 0.5\text{H}_2\text{O}$**

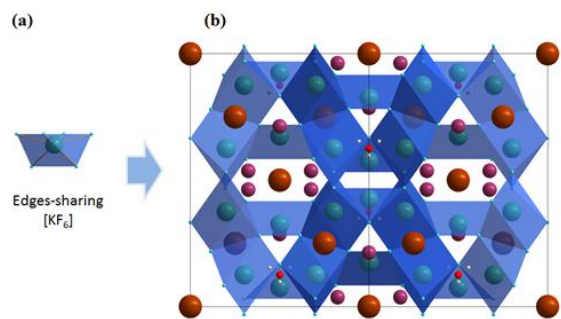
	U11	U22	U33	U23	U13	U12
Sn(1)	63(1)	63(1)	63(1)	3(1)	-3(1)	3(1)
F(1)	77(3)	67(5)	77(3)	1(3)	3(4)	1(3)
I(1)	79(1)	79(1)	79(1)	-9(1)	-9(1)	-9(1)
O(1)	26(7)	26(7)	26(7)	0	0	0
K(1)	104(3)	104(3)	146(6)	0	0	8(4)

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15 **Supplementary Table 4. Bond lengths [Å] and angles [deg.] for $\text{K}_6\text{Sn}_4\text{F}_{12}\text{I}_2 \cdot 0.5\text{H}_2\text{O}$**

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)		

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