

Supporting Information for

Large positive thermal expansion and small band-gap in double- ReO_3 type compound NaSbF_6

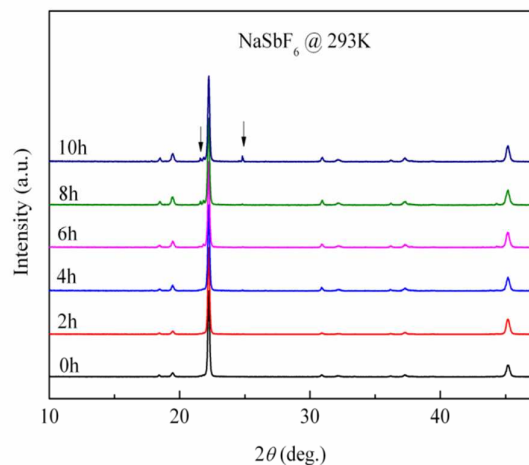


Figure S1. XRD patterns of NaSbF_6 sample exposed in air (293 K) for different durations. The arrows indicate diffractions from $\text{NaSbF}_6 \cdot n\text{H}_2\text{O}$ after a 6-hour exposure in air.

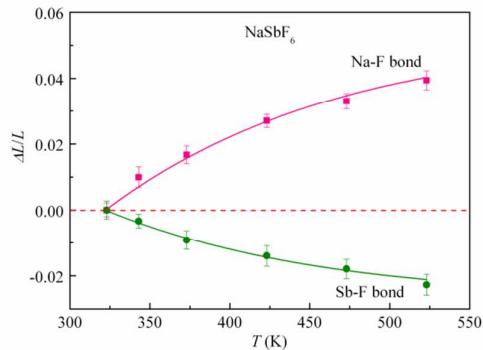


Figure S2. Variations of the apparent Na-F and Sb-F bond lengths on heating from analyses of XRD data.

Table S1. Calculated vibrational frequencies of NaSbF₆ at the Γ - point of the Brillouin Zone

Frequency (cm ⁻¹)	Symmetry	Infrared/Raman active
147.6	F_{2u}	None
176.7	F_{1u}	I
247.8	F_{2g}	R
261.3	F_{1u}	I
541.4	E_g	R
637.1	A_{1g}	R
648.9	F_{1u}	I