

Electronic Supplementary Information

Sn₁₄O₁₁Br₆: A promising birefringent material with [Sn₁₄O₁₁Br₆] layer

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Table S2. Atomic coordinates and equivalent isotropic displacement parameter for Sn₁₄O₁₁Br₆.

Atoms	<i>x</i>	<i>y</i>	<i>z</i>	$U_{(eq)}^*$
Sn1	7363(1)	902(1)	7474(1)	15(1)
Sn2	5645(1)	7944(1)	7486(1)	16(1)
Sn3	1691(1)	9127(1)	7497(1)	15(1)
Sn4	335(1)	6195(1)	7538(1)	16(1)
Sn5	8552(1)	3693(1)	7466(1)	14(1)
Sn6	3117(1)	2228(1)	7536(1)	14(1)
Sn7	4263(1)	5364(1)	6675(1)	20(1)
Sn8	4622(1)	4682(1)	8325(1)	21(1)
Sn9	1782(1)	3042(1)	9290(1)	20(1)
Sn10	8338(1)	2708(1)	5721(1)	18(1)
Sn11	9052(1)	1275(1)	9211(1)	18(1)
Sn12	12880(1)	3(1)	5730(1)	20(1)
Sn13	11090(1)	4503(1)	5791(1)	18(1)
Sn14	3622(1)	8507(1)	9256(1)	18(1)
O1	3821(5)	8146(5)	8213(2)	15(1)
O2	5904(5)	5451(5)	7487(2)	12(1)
O3	10792(5)	2318(5)	5969(2)	17(1)
O4	3514(5)	8766(5)	6779(2)	15(1)
O5	1961(5)	3918(5)	8248(2)	14(1)
O6	1458(5)	11025(5)	9024(2)	16(1)
O7	4882(5)	3117(5)	7505(2)	14(1)
O8	2566(5)	6470(5)	7507(2)	13(1)
O9	7722(6)	2679(5)	6757(2)	16(1)
O10	8064(5)	2051(5)	8181(2)	15(1)
O11	1641(5)	4500(5)	6819(2)	15(1)
Br1	5541(1)	10258(1)	9032(1)	24(1)
Br2	10019(1)	-993(1)	5972(1)	24(1)
Br3	-1868(1)	5030(1)	9021(1)	25(1)
Br4	7467(1)	6426(1)	5979(1)	25(1)
Br5	10666(1)	-2299(1)	9016(1)	24(1)
Br6	14803(1)	1628(1)	5977(1)	25(1)

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

Table S3. Selected bond lengths [\AA] and angles [deg] for $\text{Sn}_{14}\text{O}_{11}\text{Br}_6$.

Sn1-O9	2.139(4)	Sn8-O8	2.226(4)
Sn1-O10	2.133(4)	Sn8-O2	2.239(4)
Sn1-O7	2.180(4)	Sn8-O7	2.242(4)
Sn2-O4	2.131(4)	Sn9-O5	2.104(4)
Sn2-O1	2.143(4)	Sn9-O6 ^{#1}	2.153(4)
Sn2-O2	2.183(4)	Sn9-Br3	2.912(9)
Sn3-O4	2.107(4)	Sn10-O9	2.094(4)
Sn3-O1	2.115(4)	Sn10-O3	2.145(4)
Sn3-O8	2.155(4)	Sn10-Br2	2.910(8)
Sn4-O11	2.147(4)	Sn11-O10	2.074(4)
Sn4-O5	2.135(4)	Sn11-O6 ^{#2}	2.141(4)
Sn4-O8	2.186(4)	Sn11-Br5	2.942(8)
Sn5-O9	2.113(4)	Sn12-O4 ^{#4}	2.111(4)
Sn5-O10	2.111(4)	Sn12-O3	2.155(4)
Sn5-O2	2.152(4)	Sn12-Br6	2.907(8)
Sn6-O5	2.112(4)	Sn13-O11 ^{#3}	2.067(4)
Sn6-O11	2.113(4)	Sn13-O3	2.138(4)
Sn6-O7	2.146(4)	Sn13-Br4	2.943(8)
Sn7-O7	2.245(4)	Sn14-O1	2.101(4)
Sn7-O8	2.233(4)	Sn14-O6	2.150(4)
Sn7-O2	2.229(4)	Sn14-Br1	2.916(8)
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O9-Sn1-O7	82.96(16)	O2-Sn8-O7	75.22(14)
O10-Sn1-O7	82.17(16)	O8-Sn8-O2	75.26(15)
O10-Sn1-O9	79.56(15)	O8-Sn8-O7	75.59(14)
O1-Sn2-O2	82.27(15)	O5-Sn9-O6 ^{#1}	93.30(16)
O4-Sn2-O1	80.16(16)	O5-Sn9-Br3	88.19(12)
O4-Sn2-O2	82.59(15)	O6 ^{#1} -Sn9-Br3	83.40(11)
O1-Sn3-O8	83.09(15)	O3-Sn10-Br2	84.74(11)
O4-Sn3-O1	81.36(16)	O9-Sn10-O3	93.97(17)
O4-Sn3-O8	84.11(16)	O9-Sn10-Br2	88.84(11)
O5-Sn4-O8	82.83(15)	O6 ^{#2} -Sn11-Br5	84.82(11)
O5-Sn4-O11	79.70(15)	O10-Sn11-O6 ^{#2}	96.98(16)

Symmetry transformations used to generate equivalent atoms:

#1 $x, y - 1, z$ #2 $x + 1, y - 1, z$ #3 $x + 1, y, z$
#4 $x - 1, y + 1, z$ #5 $x, y + 1, z$ #6 $x - 1, y, z$

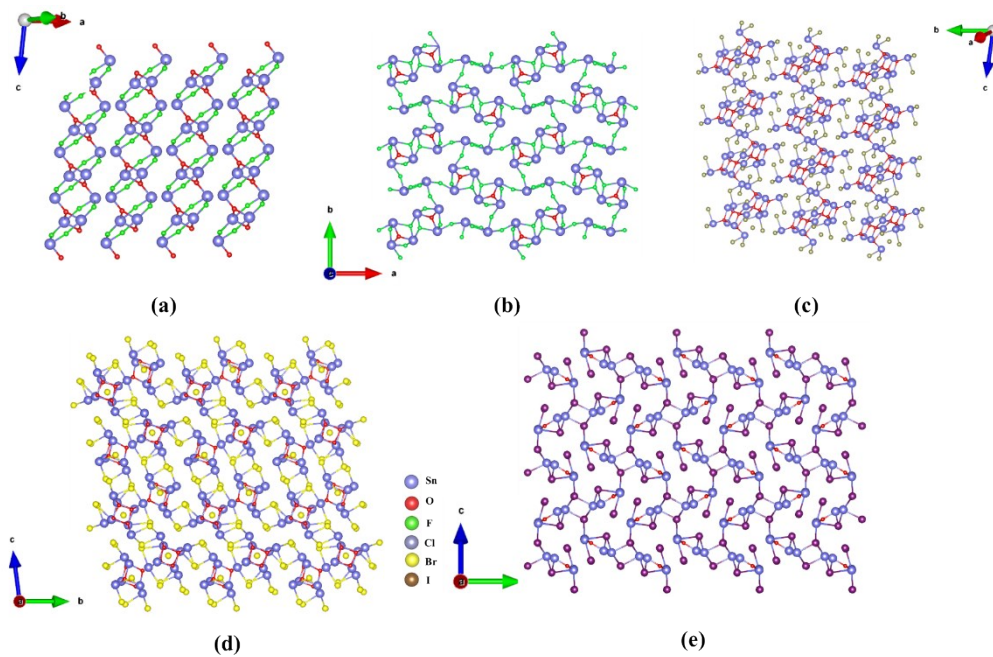


Figure S1 (a) $[\text{Sn}_4\text{O}_2\text{F}_4]$ infinite chains of $\text{Sn}_2(\text{SnOF}_2)_2$; (b) 3D $[\text{Sn}_4\text{OF}_6]$ framework of Sn_4OF_6 ; (c) $[\text{Sn}_{14}\text{O}_8\text{Cl}_{10}]$ infinite chains of $\text{Sn}_7\text{O}_4\text{Cl}_6$; (d) 3D $[\text{Sn}_7\text{O}_4\text{Br}_6]$ framework of $\text{Sn}_7\text{O}_4\text{Br}_6$; (e) 3D $[\text{Sn}_4\text{OI}_6]$ framework of Sn_4OI_6 .

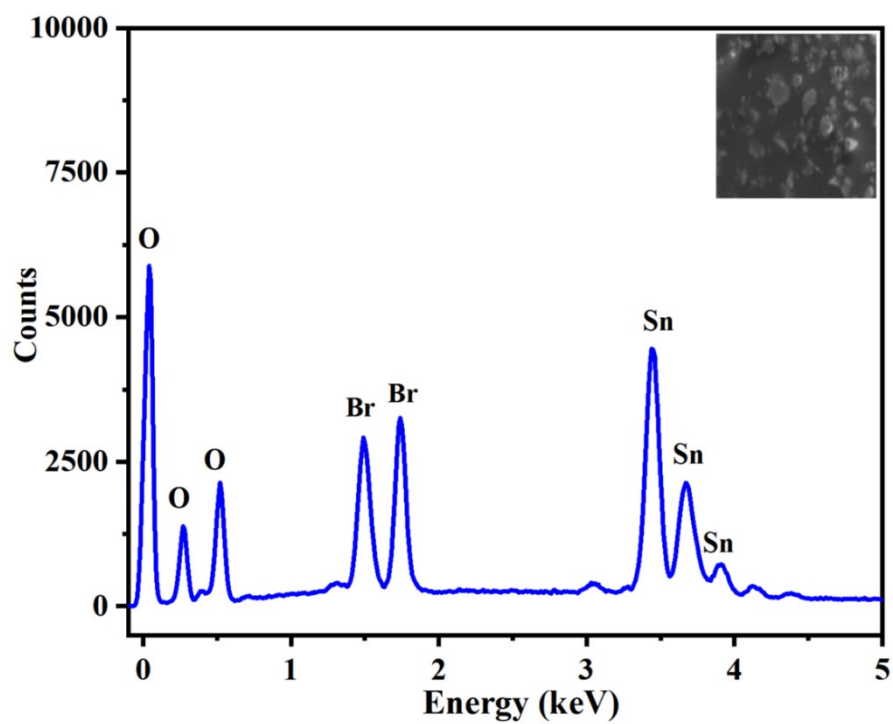
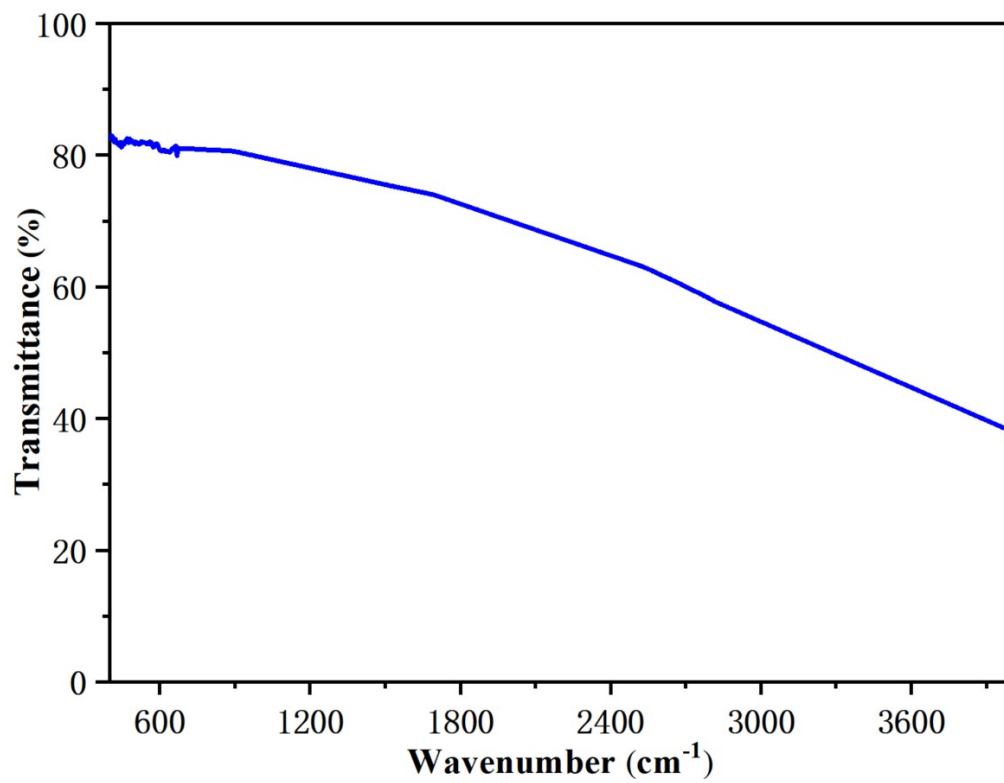


Figure S2 EDX analysis of $\text{Sn}_{14}\text{O}_{11}\text{Br}_6$.



e S3 IR Spectroscopy of Sn₁₄O₁₁Br₆.

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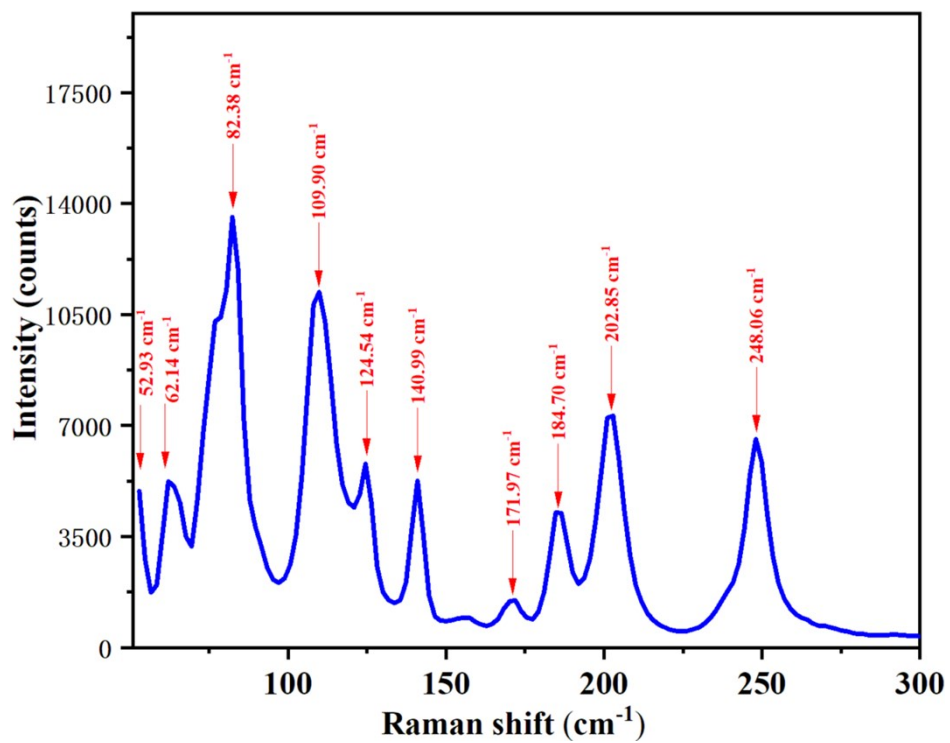


Figure S4 Raman spectroscopy of Sn₁₄O₁₁Br₆.

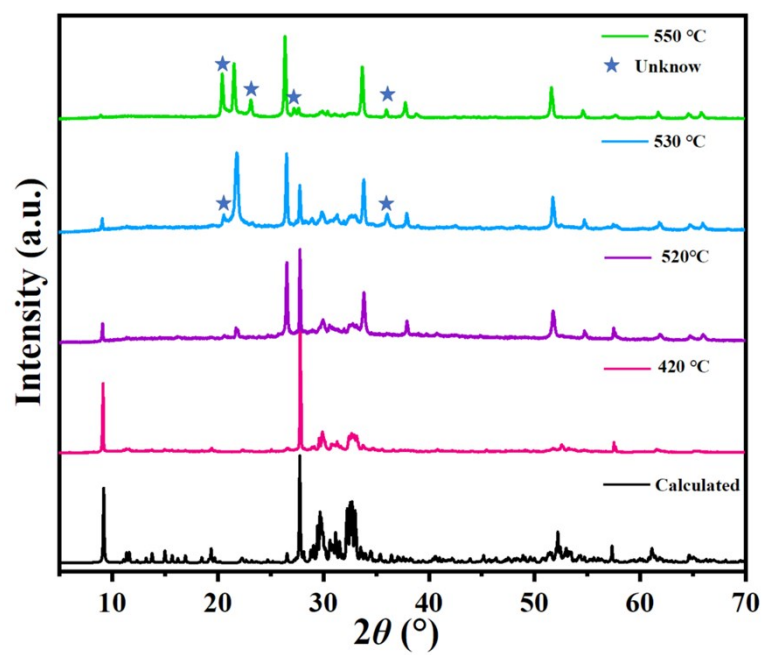


Figure S5 Powder XRD patterns of $\text{Sn}_{14}\text{O}_{11}\text{Br}_6$ at 420, 520, 530 and 550 °C, respectively.

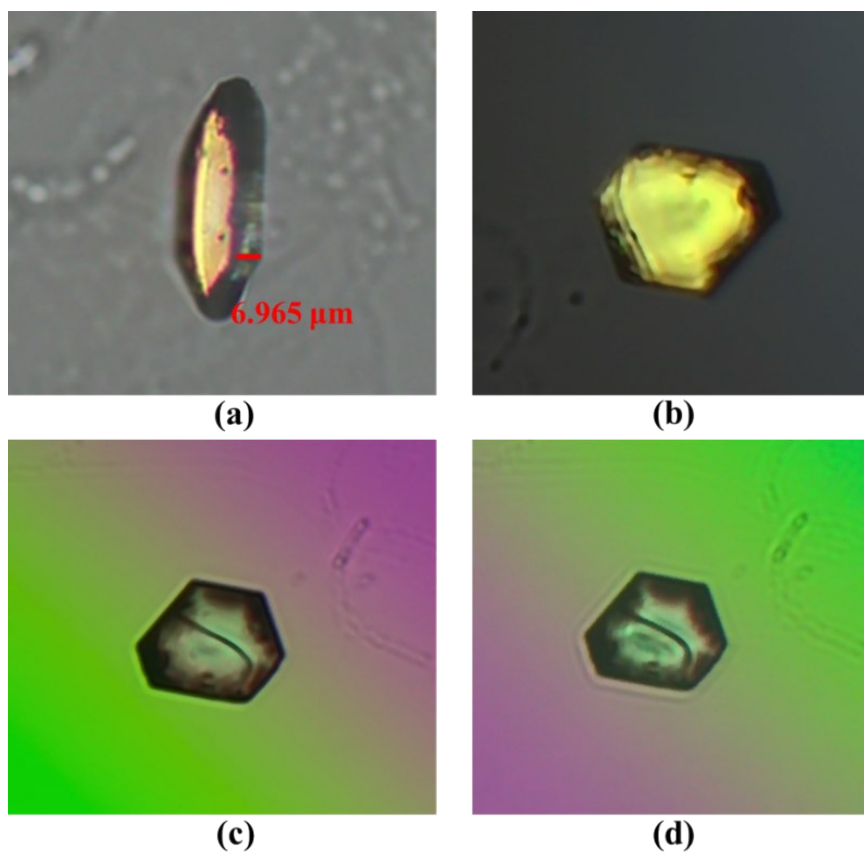


Figure S6 (a) A plate-shaped TOB crystal with a thickness of 6.965 μm; (b) The interference color of TOB crystal under the polarizing microscope; The TOB crystal in the left (c) and right (d) subtraction position.

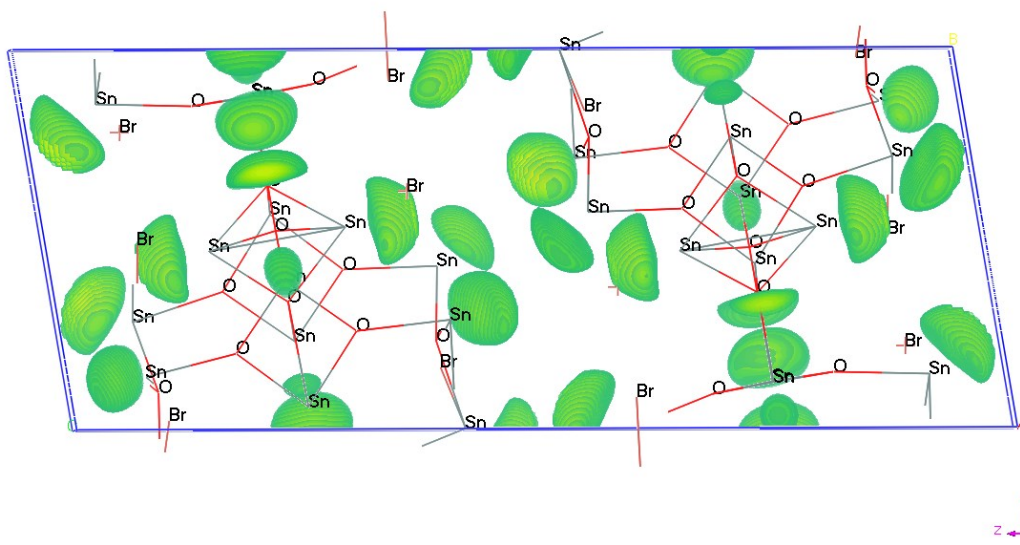


Figure S7 Electron localization function diagrams of the Sn-O/Br polyhedra in TOB.