

Electronic Supporting Information

RbSb(SO₄)(H₂PO₂)F: A Short-Wave UV Antimony(III) Oxysalt with Mixed-Anions Demonstrating Enhanced Birefringence

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Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $\text{RbSb}(\text{SO}_4)(\text{H}_2\text{PO}_2)\text{F}$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

atom	x	y	z	$U_{eq}(\text{\AA}^2)$
Sb(1)	6338.6(2)	7500	7725.8(3)	16.59(11)
Rb(1)	4266.9(3)	2500	7207.7(4)	29.79(13)
S(1)	6573.3(5)	2500	5579.2(9)	16.97(18)
P(1)	6538.4(6)	12500	9969.6(9)	17.7(2)
O(1)	5065.8(14)	7500	7708(2)	25.5(5)
O(2)	6096.6(13)	10165(3)	9456(2)	29.9(4)
O(3)	7308.1(17)	2500	6645(3)	30.0(6)
O(4)	6860(2)	2500	4032(3)	45.0(8)

Table S2. Selected Bond lengths [Å] and angles [°] for RbSb(SO₄)(H₂PO₂)F.

Sb(1)—Rb(1) ¹	4.1736(4)	Rb(1)—Sb(1)—Rb(1) ¹	81.489(9)
Sb(1)—Rb(1)	4.1736(4)	O(4) ⁸ —Rb(1)—O(1) ²	113.67(4)
Sb(1)—F(1)	1.922(2)	O(4) ⁹ —Rb(1)—O(1) ⁵	122.20(5)
Sb(1)—O(1) ²	2.1462(18)	F(1) ³ —Rb(1)—F(1)	129.48(8)
Sb(1)—O(4) ²	2.3179(19)	F(1)—Rb(1)—O(1) ⁴	62.78(5)
Rb(1)—O(3) ⁷	4.1736(4)	F(1) ³ —Rb(1)—O(1) ⁴	109.12(5)
Rb(1)—O(3) ⁸	4.1736(4)	O(4) ¹⁰ —Rb(1)—O(4) ⁹	65.78(6)
Rb(1)—O(4) ⁹	1.922(2)	O(4)—Rb(1)—O(4) ⁹	87.77(4)
Rb(1)—O(4) ⁷	2.1462(18)	O(4) ⁹ —Rb(1)—O(4) ⁸	58.29(7)
Rb(1)—O(4) ¹⁰	2.1462(18)	Rb(1) ⁷ —S(1)—Rb(1) ⁸	88.785(18)
Rb(1)—F(1) ³	3.0121(10)	Rb(1)—S(1)—Rb(1) ⁸	86.741(16)
Rb(1)—O(1) ⁴	3.3462(19)	O(2)—S(1)—Rb(1) ⁸	131.35(5)
Rb(1)—O(1) ⁵	3.3462(19)	O(2)—S(1)—Rb(1)	116.95(12)
Rb(1)—O(2) ⁶	3.129(3)	O(2)—S(1)—Rb(1) ⁷	131.35(5)
S(1)—O(4)	1.4897(19)	O(1) ¹² —P(1)—Rb(1) ⁵	130.28(8)
S(1)—O(2)	1.459(3)	O(1)—P(1)—Rb(1) ¹¹	130.28(8)
S(1)—O(3)	1.441(3)	O(1)—P(1)—Rb(1) ⁵	57.77(8)
S(1)—O(4)	1.4897(19)	O(1)—P(1)—O(1) ¹²	115.14(17)
P(1)—O(1) ¹¹	1.5071(18)	S(1)—O(2)—Rb(1) ¹³	158.53(17)
P(1)—O(1)	1.5071(19)	Rb(1)—F(1)—Rb(1) ¹	129.48(8)

Symmetry codes: (1) +X, 1+Y, +Z; (2) +X, 3/2-Y, +Z; (3) +X, -1+Y, +Z; (4) 1-X, -1/2+Y, 2-Z; (5) 1-X, 1-Y, 2-Z; (6) -1/2+X, +Y, 3/2-Z; (7) 1-X, -Y, 1-Z; (8) 1-X, 1-Y, 1-Z; (9) 1-X, -1/2+Y, 1-Z; (10) +X, 1/2-Y, +Z; (11) 1-X, 2-Y, 2-Z; (12) +X, 5/2-Y, +Z; (13) 1/2+X, +Y, 3/2-Z.

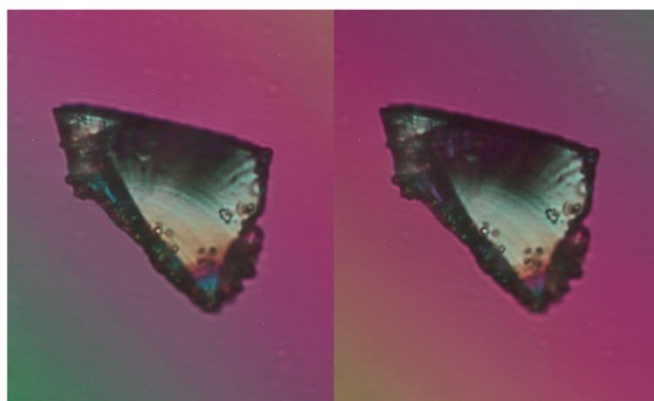


Fig. S1 The extinction diagram of $\text{RbSb}(\text{SO}_4)(\text{H}_2\text{PO}_2)\text{F}$ during the birefringence test.