

Supporting Information

Synthesis, Crystal Structure, and Optical Properties of α -SrHfS₃

K. Arun Joshi Reddy, Subhendu Jana, Sweta Yadav, and Paul A. Maggard*

Department of Chemistry and Biochemistry, Baylor University, Waco, Texas, USA, 76706

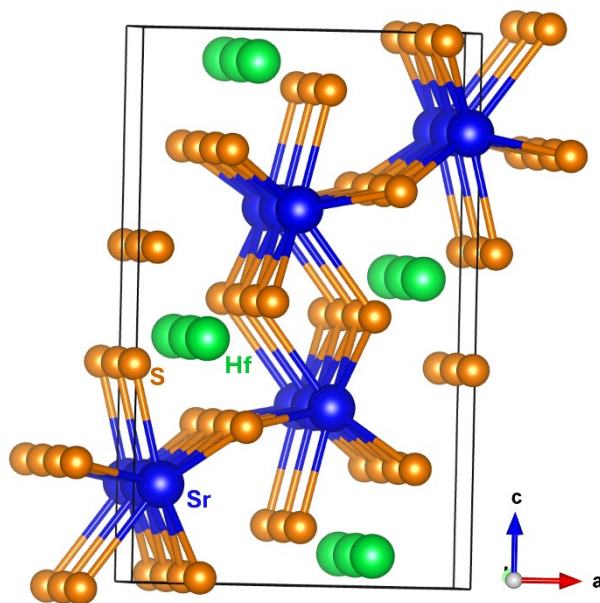


Figure S1. Unit cell view of α -SrHfS₃ crystal structure having only Sr polyhedra represented approximately along the b-axis.

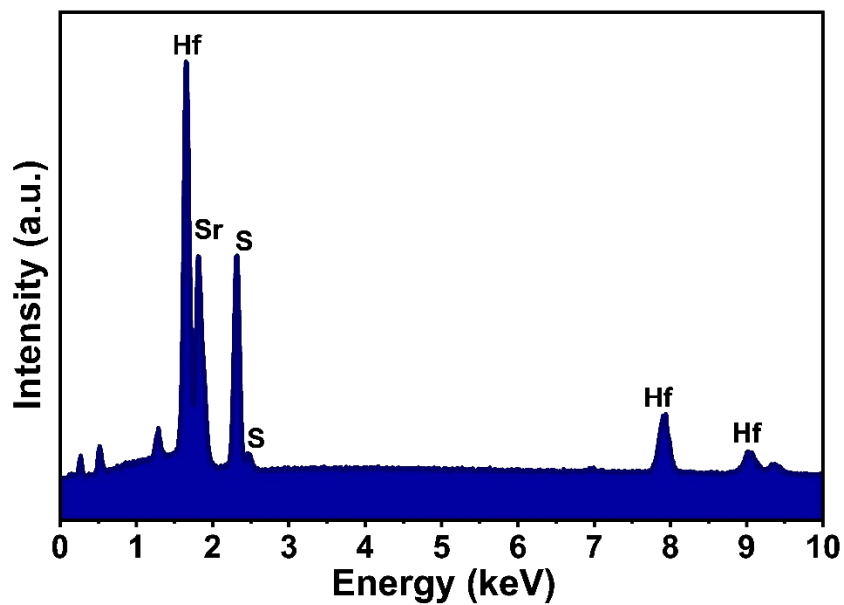


Figure S2. Energy dispersive X-ray spectroscopy (EDS) data of α -SrHfS₃ crystals showing the presence of Sr, Hf, and S atoms in the approximate molar ratio of 1:1:3.

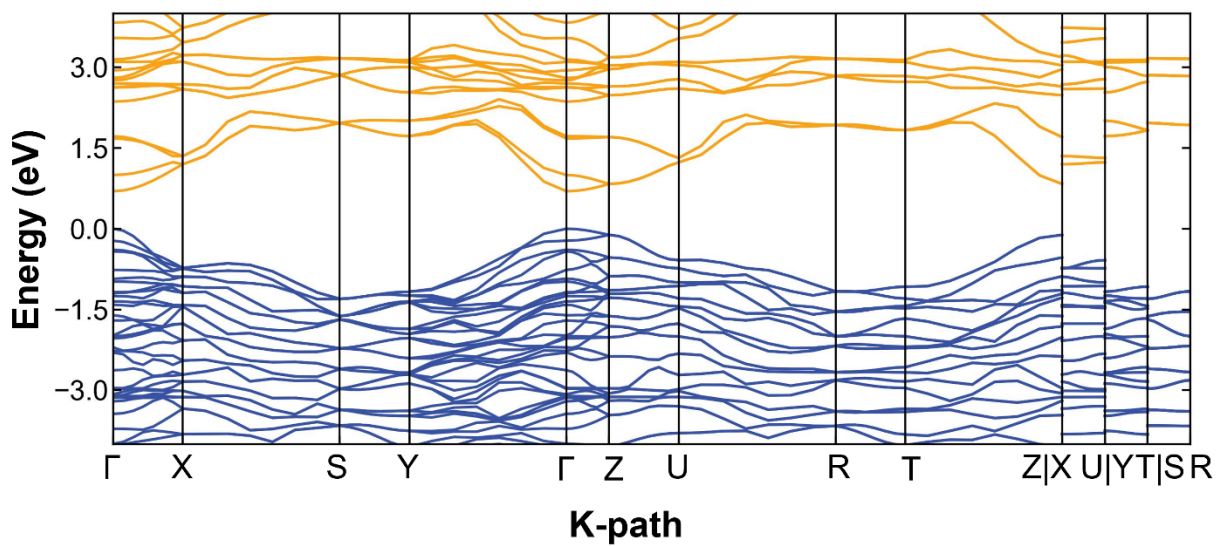


Figure S3. Electronic band structure for α -SrHfS₃.

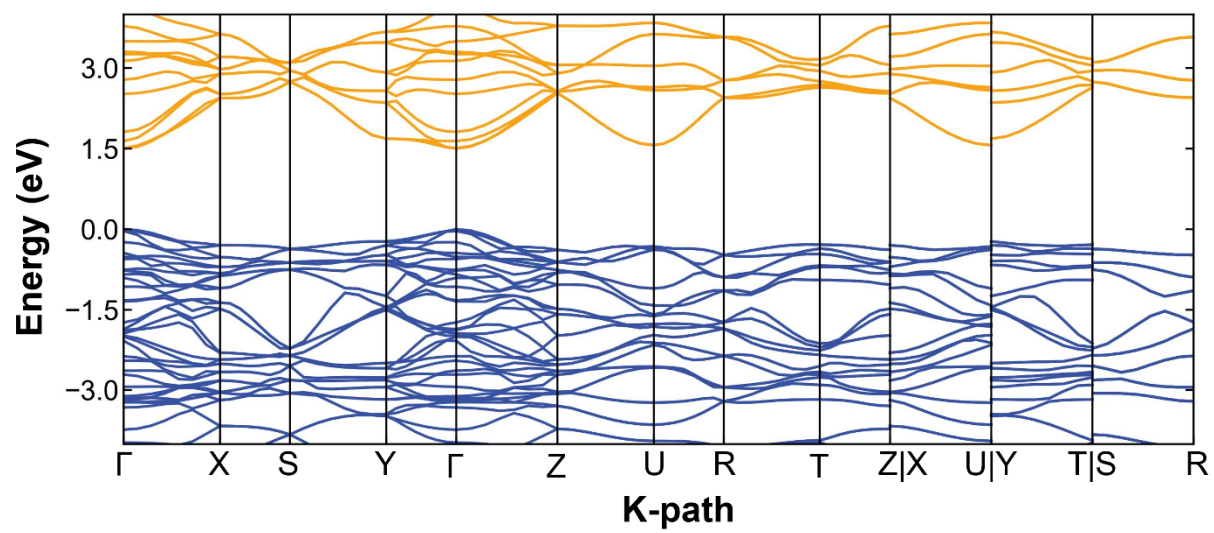


Figure S4. Electronic band structure for β -SrHfS₃.

Table S1. Atomic displacement parameters ($\text{\AA}^2$) for α -SrHfS₃.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hf1	0.01019(13)	0.00811(12)	0.00986(13)	0.000	0.00094 (6)	0.000
Sr2	0.0157(3)	0.0083(2)	0.0129(2)	0.000	-0.00040(16)	0.000
S1	0.0101(5)	0.0071(5)	0.0091(5)	0.000	0.0010(4)	0.000
S3	0.0114(5)	0.0095(5)	0.0100(5)	0.000	0.0021(4)	0.000
S2	0.0098(6)	0.0072(5)	0.0133(5)	0.000	0.0020(4)	0.000

Table S2. Geometric parameters ($\text{\AA}$, $^\circ$) for α -SrHfS₃.

Hf1—S3	2.4256 (12)	Sr2—S3 ⁱⁱ	3.0797 (11)
Hf1—S2 ⁱ	2.5525 (8)	Sr2—S3 ⁱ	3.0797 (11)
Hf1—S2 ⁱⁱ	2.5525 (8)	Sr2—S1 ^{vii}	3.0835 (13)
Hf1—S1 ⁱⁱⁱ	2.5800 (8)	Sr2—S2 ⁱⁱ	3.1062 (11)
Hf1—S1 ^{iv}	2.5800 (8)	Sr2—S2 ⁱ	3.1062 (10)
Hf1—S1	2.6066 (12)	Sr2—S2 ^{viii}	3.2871 (13)
Hf1—Sr2	3.9646 (5)	Sr2—S1	3.6781 (13)
Sr2—S3 ^v	3.0503 (11)	Sr2—Sr2 ^{ix}	3.8004 (2)
Sr2—S3 ^{vi}	3.0503 (11)	Sr2—Sr2 ^x	3.8004 (2)
S3—Hf1—S2 ⁱ	96.12 (3)	S3 ⁱⁱ —Sr2—Sr2 ^{ix}	128.098 (16)
S3—Hf1—S2 ⁱⁱ	96.12 (3)	S3 ⁱ —Sr2—Sr2 ^{ix}	51.902 (16)
S2 ⁱ —Hf1—S2 ⁱⁱ	96.22 (4)	S1 ^{vii} —Sr2—Sr2 ^{ix}	90.0
S3—Hf1—S1 ⁱⁱⁱ	91.55 (4)	S2 ⁱⁱ —Sr2—Sr2 ^{ix}	127.715 (15)
S2 ⁱ —Hf1—S1 ⁱⁱⁱ	172.26 (4)	S2 ⁱ —Sr2—Sr2 ^{ix}	52.284 (15)
S2 ⁱⁱ —Hf1—S1 ⁱⁱⁱ	83.93 (3)	S2 ^{viii} —Sr2—Sr2 ^{ix}	90.0
S3—Hf1—S1 ^{iv}	91.55 (4)	S1—Sr2—Sr2 ^{ix}	90.0
S2 ⁱ —Hf1—S1 ^{iv}	83.93 (3)	S3 ^v —Sr2—Sr2 ^x	128.532 (17)
S2 ⁱⁱ —Hf1—S1 ^{iv}	172.26 (4)	S3 ^{vi} —Sr2—Sr2 ^x	51.469 (17)
S1 ⁱⁱⁱ —Hf1—S1 ^{iv}	94.87 (4)	S3 ⁱⁱ —Sr2—Sr2 ^x	51.902 (16)
S3—Hf1—S1	175.21 (4)	S3 ⁱ —Sr2—Sr2 ^x	128.098 (16)
S2 ⁱ —Hf1—S1	87.06 (3)	S1 ^{vii} —Sr2—Sr2 ^x	90.0
S2 ⁱⁱ —Hf1—S1	87.06 (3)	S2 ⁱⁱ —Sr2—Sr2 ^x	52.284 (15)

S1 ⁱⁱⁱ —Hf1—S1	85.22 (3)	S2 ⁱ —Sr2—Sr2 ^x	127.715 (15)
S1 ^{iv} —Hf1—S1	85.22 (3)	S2 ^{viii} —Sr2—Sr2 ^x	90.0
S3—Hf1—Sr2	120.55 (3)	S1—Sr2—Sr2 ^x	90.0
S2 ⁱ —Hf1—Sr2	51.55 (2)	Sr2 ^{ix} —Sr2—Sr2 ^x	180.00 (3)
S2 ⁱⁱ —Hf1—Sr2	51.55 (2)	S3 ^v —Sr2—Hf1	124.72 (2)
S1 ⁱⁱⁱ —Hf1—Sr2	124.63 (2)	S3 ^{vi} —Sr2—Hf1	124.72 (2)
S1 ^{iv} —Hf1—Sr2	124.63 (2)	S3 ⁱⁱ —Sr2—Hf1	92.51 (2)
S1—Hf1—Sr2	64.24 (3)	S3 ⁱ —Sr2—Hf1	92.51 (2)
S3 ^v —Sr2—S3 ^{vi}	77.06 (3)	S1 ^{vii} —Sr2—Hf1	159.04 (3)
S3 ^v —Sr2—S3 ⁱⁱ	141.332 (19)	S2 ⁱⁱ —Sr2—Hf1	40.058 (16)
S3 ^{vi} —Sr2—S3 ⁱⁱ	90.691 (10)	S2 ⁱ —Sr2—Hf1	40.058 (16)
S3 ^v —Sr2—S3 ⁱ	90.691 (10)	S2 ^{viii} —Sr2—Hf1	70.77 (2)
S3 ^{vi} —Sr2—S3 ⁱ	141.332 (19)	S1—Sr2—Hf1	39.660 (19)
S3 ⁱⁱ —Sr2—S3 ⁱ	76.20 (3)	Sr2 ^{ix} —Sr2—Hf1	90.0
S3 ^v —Sr2—S1 ^{vii}	70.12 (3)	Sr2 ^x —Sr2—Hf1	90.0
S3 ^{vi} —Sr2—S1 ^{vii}	70.12 (3)	Hf1 ⁱⁱⁱ —S1—Hf1 ^{iv}	94.87 (4)
S3 ⁱⁱ —Sr2—S1 ^{vii}	71.22 (3)	Hf1 ⁱⁱⁱ —S1—Hf1	94.78 (3)
S3 ⁱ —Sr2—S1 ^{vii}	71.22 (3)	Hf1 ^{iv} —S1—Hf1	94.78 (3)
S3 ^v —Sr2—S2 ⁱⁱ	135.22 (3)	Hf1 ⁱⁱⁱ —S1—Sr2 ^{xi}	96.31 (3)
S3 ^{vi} —Sr2—S2 ⁱⁱ	87.00 (2)	Hf1 ^{iv} —S1—Sr2 ^{xi}	96.31 (3)
S3 ⁱⁱ —Sr2—S2 ⁱⁱ	79.23 (3)	Hf1—S1—Sr2 ^{xi}	163.57 (5)
S3 ⁱ —Sr2—S2 ⁱⁱ	124.61 (3)	Hf1 ⁱⁱⁱ —S1—Sr2	132.19 (2)
S1 ^{vii} —Sr2—S2 ⁱⁱ	141.836 (16)	Hf1 ^{iv} —S1—Sr2	132.19 (2)
S3 ^v —Sr2—S2 ⁱ	87.00 (2)	Hf1—S1—Sr2	76.10 (3)
S3 ^{vi} —Sr2—S2 ⁱ	135.22 (3)	Sr2 ^{xi} —S1—Sr2	87.46 (3)
S3 ⁱⁱ —Sr2—S2 ⁱ	124.61 (3)	Hf1—S3—Sr2 ^v	99.92 (3)
S3 ⁱ —Sr2—S2 ⁱ	79.23 (3)	Hf1—S3—Sr2 ^{vi}	99.92 (3)
S1 ^{vii} —Sr2—S2 ⁱ	141.836 (16)	Sr2 ^v —S3—Sr2 ^{vi}	77.06 (3)
S2 ⁱⁱ —Sr2—S2 ⁱ	75.43 (3)	Hf1—S3—Sr2 ^{xii}	99.81 (4)
S3 ^v —Sr2—S2 ^{viii}	71.42 (3)	Sr2 ^v —S3—Sr2 ^{xii}	160.27 (4)
S3 ^{vi} —Sr2—S2 ^{viii}	71.42 (3)	Sr2 ^{vi} —S3—Sr2 ^{xii}	99.937 (11)
S3 ⁱⁱ —Sr2—S2 ^{viii}	139.139 (19)	Hf1—S3—Sr2 ^{xiii}	99.81 (4)
S3 ⁱ —Sr2—S2 ^{viii}	139.139 (19)	Sr2 ^v —S3—Sr2 ^{xiii}	99.937 (11)

S1 ^{vii} —Sr2—S2 ^{viii}	130.19 (3)	Sr2 ^{vi} —S3—Sr2 ^{xiii}	160.27 (4)
S2 ⁱⁱ —Sr2—S2 ^{viii}	63.84 (3)	Sr2 ^{xii} —S3—Sr2 ^{xiii}	76.19 (3)
S2 ⁱ —Sr2—S2 ^{viii}	63.84 (3)	Hf1 ^{xiii} —S2—Hf1 ^{xii}	96.23 (4)
S3 ^v —Sr2—S1	141.326 (17)	Hf1 ^{xiii} —S2—Sr2 ^{xiii}	88.389 (15)
S3 ^{vi} —Sr2—S1	141.326 (17)	Hf1 ^{xii} —S2—Sr2 ^{xiii}	151.97 (5)
S3 ⁱⁱ —Sr2—S1	62.11 (3)	Hf1 ^{xiii} —S2—Sr2 ^{xii}	151.97 (5)
S3 ⁱ —Sr2—S1	62.11 (3)	Hf1 ^{xii} —S2—Sr2 ^{xii}	88.389 (15)
S1 ^{vii} —Sr2—S1	119.38 (3)	Sr2 ^{xiii} —S2—Sr2 ^{xii}	75.43 (3)
S2 ⁱⁱ —Sr2—S1	62.51 (3)	Hf1 ^{xiii} —S2— Sr2 ^{xiv}	91.42 (3)
S2 ⁱ —Sr2—S1	62.51 (3)	Hf1 ^{xii} —S2—Sr2 ^{xiv}	91.42 (3)
S2 ^{viii} —Sr2—S1	110.43 (3)	Sr2 ^{xiii} —S2— Sr2 ^{xiv}	116.16 (3)
S3 ^v —Sr2—Sr2 ^{ix}	51.469 (17)	Sr2 ^{xii} —S2—Sr2 ^{xiv}	116.16 (3)
S3 ^{vi} —Sr2—Sr2 ^{ix}	128.532 (17)		

Symmetry codes: (i) -x+1/2, -y+1, z+1/2; (ii) -x+1/2, -y, z+1/2; (iii) -x, -y, -z+1; (iv) -x, -y+1, -z+1; (v) -x+1, -y+1, -z+1; (vi) -x+1, -y, -z+1; (vii) x+1/2, y, -z+3/2; (viii) x+1/2, y, -z+1/2; (ix) x, y+1, z; (x) x, y-1, z; (xi) x-1/2, y, -z+3/2; (xii) -x+1/2, -y, z-1/2; (xiii) -x+1/2, -y+1, z-1/2; (xiv) x-1/2, y, -z+1/2.

Table S3. Calculated bond valence sums for the ions in α -SrHfS₃

Atom	BVS
Sr1	2.02
Hf1	3.95
S1	2.02
S2	1.94
S3	2.02