

Supporting information

Synthesis and physical properties of the oxofluoride $\text{Cu}_2(\text{SeO}_3)\text{F}_2$

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Table S1

Atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for $\text{Cu}_2\text{SeO}_3\text{F}_2$.

Atom	x	y	z	U(eq)
Se(1)	0.29659(6)	0.7500	0.16062(8)	0.00537(9)
Cu(1)	0.40025(5)	0.43124(4)	0.24699(6)	0.00549(8)
F(1)	0.1510(2)	0.43748(18)	0.1044(3)	0.0095(3)
O(1)	0.1566(4)	0.7500	-0.0996(6)	0.0088(6)
O(2)	0.4467(3)	0.6167(2)	0.1000(4)	0.0067(4)

Table S2Selected bond Lengths (Å) and Angles (°) for Cu₂SeO₃F₂

Se1—O1	1.753(3)	Cu1—O2 ^{iv}	2.260(2)
Se1—O2	1.695(2)	Cu1—F1 ⁱⁱⁱ	2.381(2)
Se1—O2 ⁱ	1.695(2)	F1—Cu1 ^v	1.9562(2)
Cu1—F1	1.933(2)	F1—Cu1 ^{vi}	2.381(2)
Cu1—F1 ⁱⁱ	1.956(2)	O1—Cu1 ^{vi}	1.978(1)
Cu1—O1 ⁱⁱⁱ	1.978(1)	O1—Cu1 ^{vii}	1.978(1)
Cu1—O2	1.985(2)	O2—Cu1 ^{iv}	2.260(2)
O2 ⁱ —Se1—O2	97.92(14)	F1 ⁱⁱ —Cu1—F1 ⁱⁱⁱ	76.62(7)
O2 ⁱ —Se1—O1	100.88(9)	O1 ⁱⁱⁱ —Cu1—F1 ⁱⁱⁱ	94.21(9)
O2—Se1—O1	100.88(9)	O2—Cu1—F1 ⁱⁱⁱ	83.99(7)
F1—Cu1—F1 ⁱⁱ	176.39(10)	O2 ^{iv} —Cu1—F1 ⁱⁱⁱ	153.33(7)
F1—Cu1—O1 ⁱⁱⁱ	91.1(1)	Cu1—F1—Cu1 ^v	130.61(10)
F1 ⁱⁱ —Cu1—O1 ⁱⁱⁱ	91.63(10)	Cu1—F1—Cu1 ^{vi}	119.86(8)
F1—Cu1—O2	87.34(8)	Cu1 ^v —F1—Cu1 ^{vi}	103.38(7)
F1 ⁱⁱ —Cu1—O2	89.83(8)	Se1—O1—Cu1 ^{vi}	118.10(8)
O1 ⁱⁱⁱ —Cu1—O2	177.35(9)	Se1—O1—Cu1 ^{vii}	118.10(8)
F1—Cu1—O2 ^{iv}	95.27(7)	Cu1 ^{vi} —O1—Cu1 ^{vii}	123.01(16)
F1 ⁱⁱ —Cu1—O2 ^{iv}	86.20(7)	Se1—O2—Cu1	119.38(10)
O1 ⁱⁱⁱ —Cu1—O2 ^{iv}	106.68(9)	Se1—O2—Cu1 ^{iv}	128.53(11)
O2—Cu1—O2 ^{iv}	75.61(9)	Cu1—O2—Cu1 ^{iv}	104.39(9)
F1—Cu1—F1 ⁱⁱⁱ	100.82(5)		

Note. Symmetry transformations used to generate equivalent atoms:

- (i) $x, 1.5-y, z$; (ii) $0.5+x, y, 0.5-z$; (iii) $0.5-x, 1-y, 0.5+z$; (iv) $1-x, 1-y, -z$; (v) $-0.5+x, y, 0.5-z$;
 (vi) $0.5-x, 1-y, -0.5+z$; (vii) $0.5-x, 0.5+y, -0.5+z$.

Table S3Bond valence sum (BVS) calculation results for $\text{Cu}_2\text{SeO}_3\text{F}_2$

<u>Atoms</u>	<u>Bonding Distance</u>	<u>Bond Valence</u>	<u>Atoms</u>	<u>Bonding Distance</u>	<u>Bond Valence</u>
Se1—O1	1.753(3)	1.17	O1—Cu ^{iv}	1.9777(15)	0.41
Se1—O2	1.695(2)	1.37	O1—Cu ^{vii}	1.9777(15)	0.41
Se1—O2 ⁱ	1.695(2)	1.37	O1—Se1	1.753(3)	1.17
		3.9			2.0
Cu1—F1	1.933(2)	0.4	O2—Cu1	1.985(2)	0.4
Cu1—F1 ⁱⁱ	1.956(2)	0.37	O2—Cu1 ^{iv}	2.260(2)	0.2
Cu1—F1 ⁱⁱⁱ	2.381(2)	0.12	O2—Se1	1.695(2)	1.37
Cu1—O1 ⁱⁱⁱ	1.978(1)	0.41			1.97
Cu1—O2	1.985(2)	0.40	F1—Cu1 ^{vi}	1.978(1)	0.35
Cu1—O2 ^{iv}	2.260(2)	0.20	F1—Cu1 ^{vii}	1.978(1)	0.35
		1.9	F1—Cu1	1.933(2)	0.4
					1.1

Note. The R_o values that were used for the bond valence (BVS) calculations are: 1.811 for Se—O bonds, 1.73 for Se—F bonds, 1.649 for Cu—O bonds and 1.594 for Cu—F bonds.²²

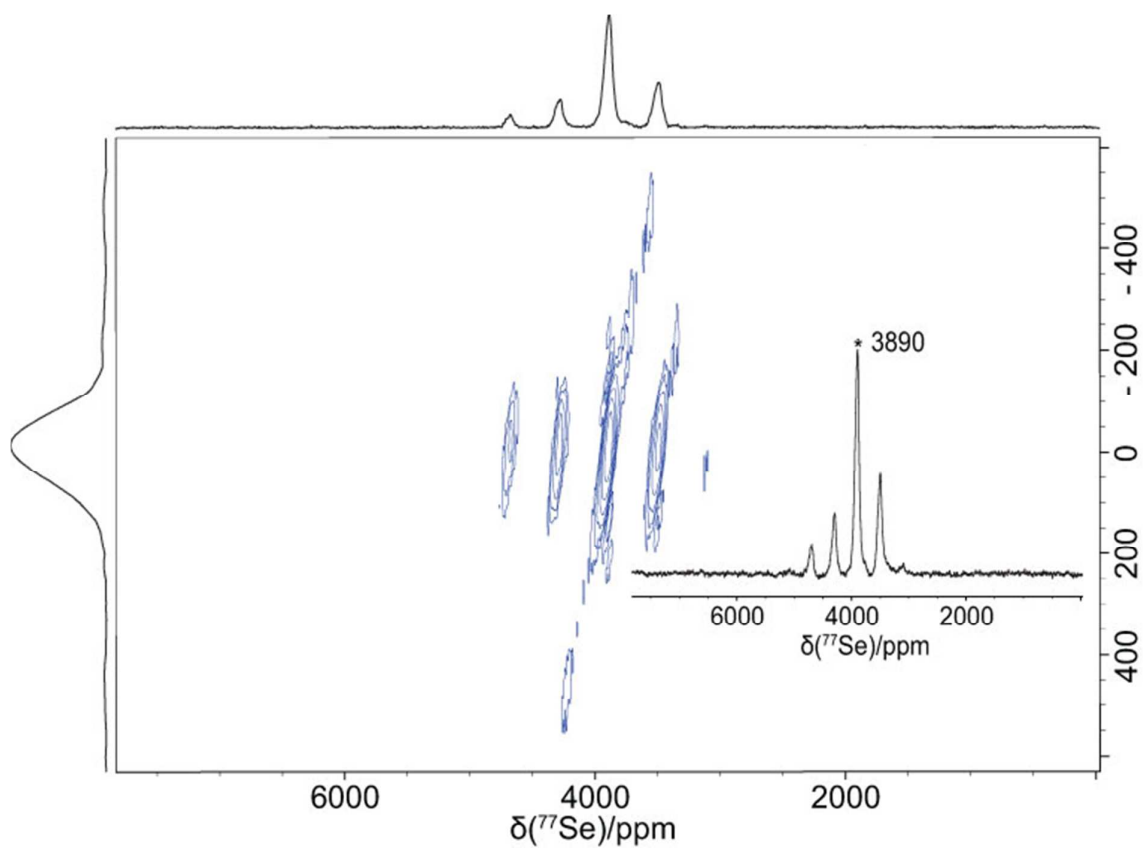


Figure S1 ^{77}Se aMAT spectrum of the $\text{Cu}_2\text{SeO}_3\text{F}_2$ crystals, confirming the presence of a single resonance with an isotropic shift of 3890 ppm.