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Supplementary material

Synthesis and crystal structure of two synthetic oxofluoride framework compounds – $Co_2TeO_3F_2$ and $Co_2SeO_3F_2$

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Table S1-1

Atomic coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for $Co_2TeF_2O_3$.

Atom	*X*	*Y*	*z*	*U*(eq)
Te(1)	0.69889(7)	¼	0.18293(9)	0.00634(16)
Co(1)	0.58538(10)	0.56678(7)	0.24427(13)	0.0070(2)
F(1)	0.6619(4)	0.4566(3)	0.5749(6)	0.0119(7)
O(1)	0.6487(7)	¾	0.3931(11)	0.0108(12)
O(2)	0.5410(5)	0.3830(4)	0.0861(7)	0.0082(8)

Table S1-2

Atomic coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for $Co_2SeF_2O_3$.

Atom	*X*	*Y*	*z*	*U*(eq)
Se(1)	0.68383(15)	¼	0.1481(2)	0.0111(3)
Co(1)	0.59148(13)	0.56454(10)	0.2482(2)	0.0077(3)
F(1)	0.6600(5)	0.4535(5)	0.5746(7)	0.0138(10)
O(1)	0.6645(10)	¾	0.3949(11)	0.0097(17)
O(2)	0.5419(6)	0.3786(5)	0.0770(9)	0.0070(12)

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

Table S2-1

Selected Bond Lengths (Å) and Angles (º) for $Co_2TeF_2O_3$.

Te1—O2^{i}	1.860(4)	Co1—F1^{ii}	2.084(3)
Te1—O2	1.860(4)	Co1—F1	2.157(3)
Te1—O1^{ii}	1.904(6)	F1—Co1^{iv}	2.075(3)
Co1—O2^{iii}	2.049(4)	F1—Co1^{v}	2.084(3)
Co1—F1^{iv}	2.075(3)	O1—Te1^{v}	1.904(6)
Co1—O2	2.078(4)	O1—Co1^{vi}	2.081(3)
Co1—O1	2.081(3)	O2—Co1^{iii}	

O2^{i}—Te1—O2	93.59(17)	F1^{iv}—Co1—F1	78.18(12)
O2^{i}—Te1—O1^{ii}	98.48(11)	O2—Co1—F1	84.25(14)
O2—Te1—O1^{ii}	98.48(11)	O1—Co1—F1	95.76(9)
O2^{iii}—Co1—F1^{iv}	91.33(14)	F1^{ii}—Co1—F1	93.22(12)
O2^{iii}—Co1—O2	78.97(15)	Co1^{iv}—F1—Co1^{v}	125.10(15)
F1^{iv}—Co1—O2	86.80(14)	Co1^{iv}—F1—Co1	101.82(13)
O2^{iii}—Co1—O1	101.66(12)	Co1^{v}—F1—Co1	130.10(15)
F1^{iv}—Co1—O1	97.21(9)	Te1^{v}—O1—Co1	116.02(2)
O2—Co1—O1	175.91(12)	Te1^{v}—O1—Co1^{vi}	116.02(2)
O2^{iii}—Co1—F1^{ii}	93.89(14)	Co1—O1—Co1^{vi}	127.70(3)
F1^{iv}—Co1—F1^{ii}	166.69(12)	Te1—O2—Co1^{iii}	134.68(21)
O2—Co1—F1^{ii}	82.19(14)	Te1—O2—Co1	116.54(20)
O1—Co1—F1^{ii}	93.73(9)	Co1^{iii}—O2—Co1	101.03(16)
O2^{iii}—Co1—F1	160.69(14)		

Table S2-2

Selected Bond Lengths (Å) and Angles (º) for $Co_2SeF_2O_3$.

Se1—O2^{i}	1.692(5)	Co1—F1^{ii}	2.039(4)
Se1—O2	1.692(5)	Co1—F1	2.130(4)
Se1—O1^{ii}	1.747(7)	F1—Co1^{iv}	2.067(4)
Co1—O2^{iii}	2.073(5)	F1—Co1^{v}	2.039(4)
Co1—F1^{iv}	2.067(4)	O1—Se1^{v}	1.747(7)
Co1—O2	2.105(5)	O1—Co1^{vi}	2.083(3)
Co1—O1	2.083(3)	O2—Co1^{iii}	2.073(5)
O2^{i}—Se1—O2	98.96(23)	F1^{iv}—Co1—F1	77.54(15)
O2^{i}—Se1—O1^{ii}	102.10(16)	O2—Co1—F1	86.39(19)
O2—Se1—O1^{ii}	102.10(16)	O1—Co1—F1	95.46(13)
O2^{iii}—Co1—F1^{iv}	89.80(17)	F1^{ii}—Co1—F1	96.96(15)
O2^{iii}—Co1—O2	78.24(19)	Co1^{iv}—F1—Co1^{v}	124.45(18)
F1^{iv}—Co1—O2	88.38(18)	Co1^{iv}—F1—Co1	102.46(17)
O2^{iii}—Co1—O1	101.06(14)	Co1^{v}—F1—Co1	128.86(19)
F1^{iv}—Co1—O1	97.45(13)	Se1^{v}—O1—Co1	116.96(3)
O2—Co1—O1	174.14(15)	Se1^{v}—O1—Co1^{vi}	116.96(3)
O2^{iii}—Co1—F1^{ii}	93.16(17)	Co1—O1—Co1^{vi}	125.85(4)
F1^{iv}—Co1—F1^{ii}	169.91(15)	Se1—O2—Co1^{iii}	133.05(27)
O2—Co1—F1^{ii}	82.80(18)	Se1—O2—Co1	117.99(26)
O1—Co1—F1^{ii}	91.45(14)	Co1^{iii}—O2—Co1	101.76(21)
O2^{iii}—Co1—F1	160.39(18)		

Note. Symmetry transformations used to generate equivalent atoms:
(i) x, 0.5-y, z; (ii) 1.5-x, 1-y, -0.5+z; (iii) 1-x, 1-y, -z; (iv) 1-x, 1-y, 1-z;
(v) 1.5-x, 1-y, 0.5+z; (vi) x, 1.5-y, z.

Table S3-1
Results from Bond Valence Sum (BVS) calculations of $Co_2TeF_2O_3$.

Atoms	Bonding distance	Bond valence	Atoms	Bonding distance	Bond valence
Te1—O1^{ii}	1.904(5)	1.2	O1—Co1	2.081(3)	0.35
Te1—O2	1.860(3)	1.4	O1—Co1^{vi}	2.081(3)	0.35
Te1—O2^{i}	1.860(3)	1.4	O1—Te1^{v}	1.904(5)	1.20
		4.0			**1.9**
Co1—O1	2.081(3)	0.35	O2—Co1	2.049(4)	0.35
Co1—O2^{iii}	2.049(4)	0.38	O2—Co1^{iii}	2.049(4)	0.35
Co1—O2	2.078(3)	0.35	O2—Te1	1.860(3)	1.30
Co1—F1^{iv}	2.075(3)	0.31			**2.0**
Co1—F1^{ii}	2.084(3)	0.30	F1—Co1^{iv}	2.075(3)	0.30
Co1—F1	2.157(3)	0.25	F1—Co1^{v}	2.084(3)	0.30
		1.9	F1—Co1	2.157(3)	0.25
					0.85

Table S3-2
Results from Bond Valence Sum (BVS) calculations of $Co_2SeF_2O_3$.

Atoms	Bonding distance	Bond valence	Atoms	Bonding distance	Bond valence
Se1—O1^{ii}	1.747(7)	1.2	O1—Co1	2.083(3)	0.35
Se1—O2	1.692(5)	1.2	O1—Co1^{vi}	2.083(3)	0.36
Se1—O2^{i}	1.692(5)	1.3	O1—Se1^{v}	1.747(7)	1.19
		3.7			**1.9**
Co1—O1	2.083(3)	0.35	O2—Co1	2.105(5)	0.33
Co1—O2^{iii}	2.073(5)	0.36	O2—Co1^{iii}	2.073(5)	0.36
Co1—O2	2.105(5)	0.33	O2—Se1	1.692(5)	1.38
Co1—F1^{iv}	2.067(4)	0.27			**2.0**
Co1—F1^{ii}	2.039(4)	0.34	F1—Co1^{iv}	2.067(4)	0.32
Co1—F1	2.130(4)	0.32	F1—Co1^{v}	2.039(4)	0.34
		1.97	F1—Co1	2.130(4)	0.27
					0.93

Note. All the calculation were made using following R_0 values: 1.977 for Te—O bonds [A], 1.811 for Se—O bonds [A], 1.692 for Co—O bonds [A] and 1.640 for Co—F bonds [B].

Symmetry transformations used to generate equivalent atoms:
(i) x, 0.5-y, z; (ii) 1.5-x, 1-y, -0.5+z; (iii) 1-x, 1-y, -z; (iv) 1-x, 1-y, 1-z;
(v) 1.5-x, 1-y, 0.5+z; (vi) x, 1.5-y, z.

References

[A] I.D. Brown and D. Altermatt, Acta Cryst. B41 (1985) 244-247.

[B] N.E. Brese and M. O'Keeffe, Acta Cryst. B47 (1991) 192-197.