Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Low temperature red luminescence of a fluorinated Mn-doped zinc selenite

Joseba Orive [a], *Rolindes Balda* [b,c], *Joaquín Fernández* [b,c], *Luis Lezama* [d] *and María I. Arriortua* [a,]*

[a] Departamento de Mineralogía y Petrología, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Apdo.644, 48080 Bilbao, Spain.

[b] Departamento Física Aplicada I, Escuela Técnica Superior de Ingeniería, Alda. Urquijo s/n 48013 Bilbao, Spain.

[c] Centro de Física de Materiales CSIC-UPV/EHU and Donostia International Physics Center, Apdo. 1072, 20080 San Sebastián, Spain.

[d] Departamento de Química Inorgánica, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Apdo.644, 48080 Bilbao, Spain.

* Corresponding author: maribel.arriortua@ehu.es

Phone: 34-946012162. Fax: 34-946013500

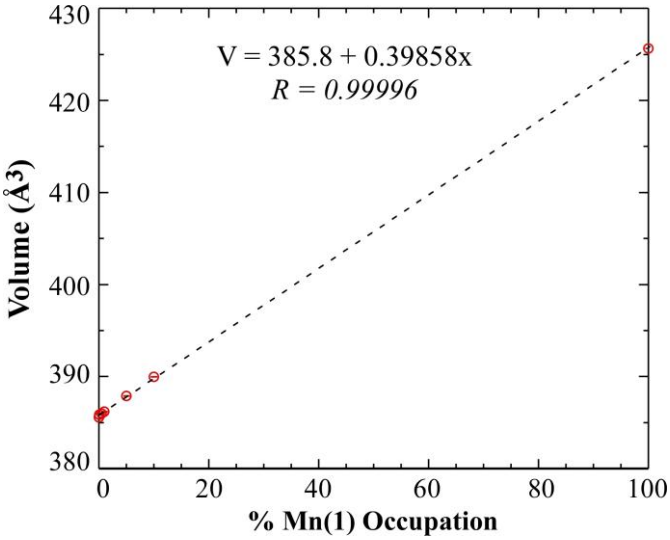


Figure S1. Variation of the volume as a function of the occupation factor of the manganese atoms for $M_2(SeO_3)F_2$ (M = Zn (**1**), Mn (**2**)) system.

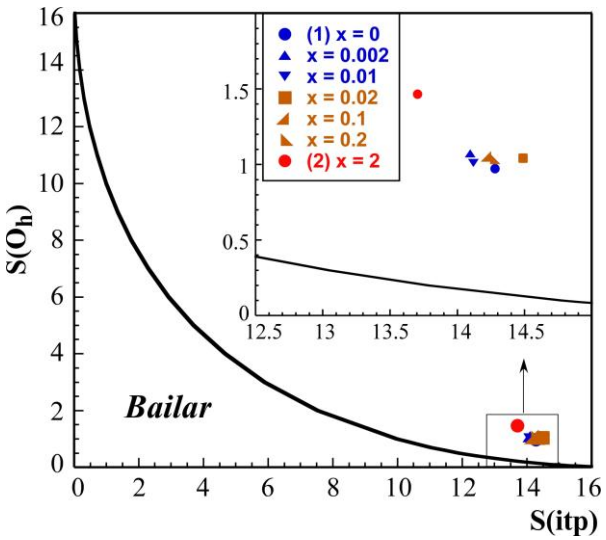


Figure S2. Distortion values of the $[(Mn,Zn)O_3F_3]$ octahedra belonging to $Zn_2(SeO_3)F_2$ (**1**), $Mn_2(SeO_3)F_2$ (**2**) and to the Mn-doped compounds.

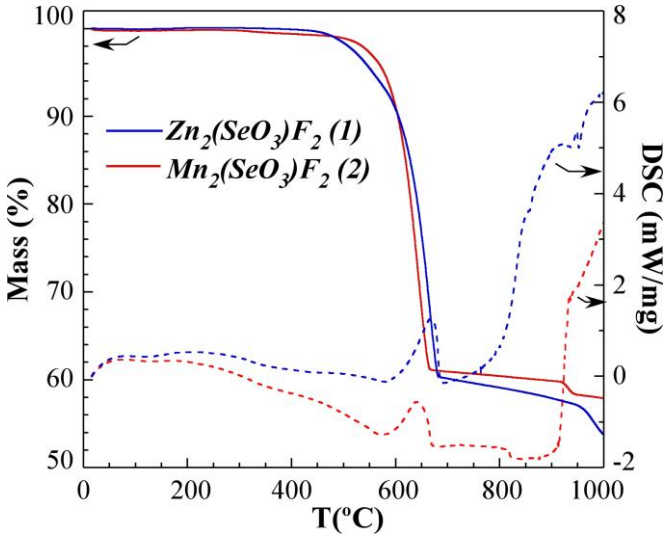


Figure S3. Thermal analysis (TGA, DSC) of $Zn_2(SeO_3)F_2$ (**1**) and $Mn_2(SeO_3)F_2$ (**2**).

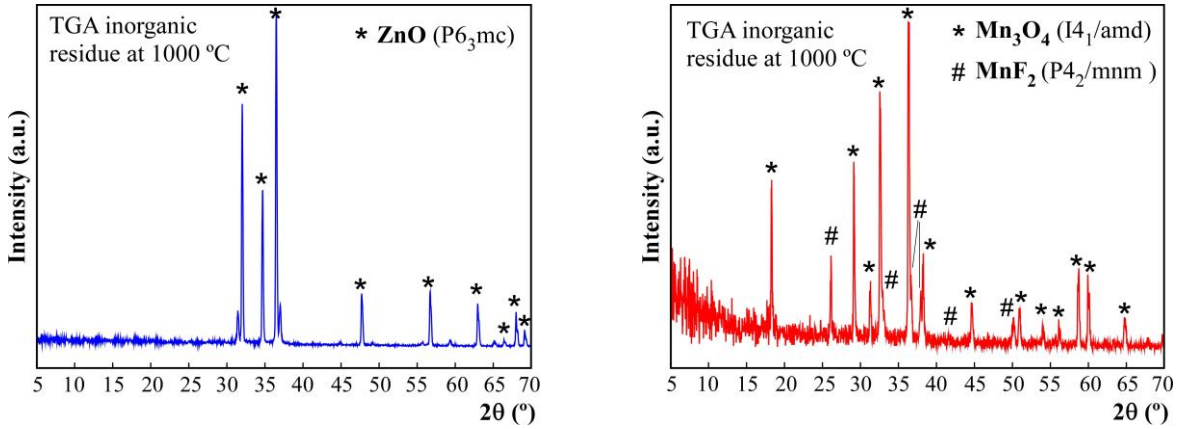


Figure S4. X-ray powder diffraction patterns of the TGA inorganic residues obtained at 1000 ºC for **(a)** $Zn_2(SeO_3)F_2$ (**1**) and **(b)** $Mn_2(SeO_3)F_2$ (**2**).

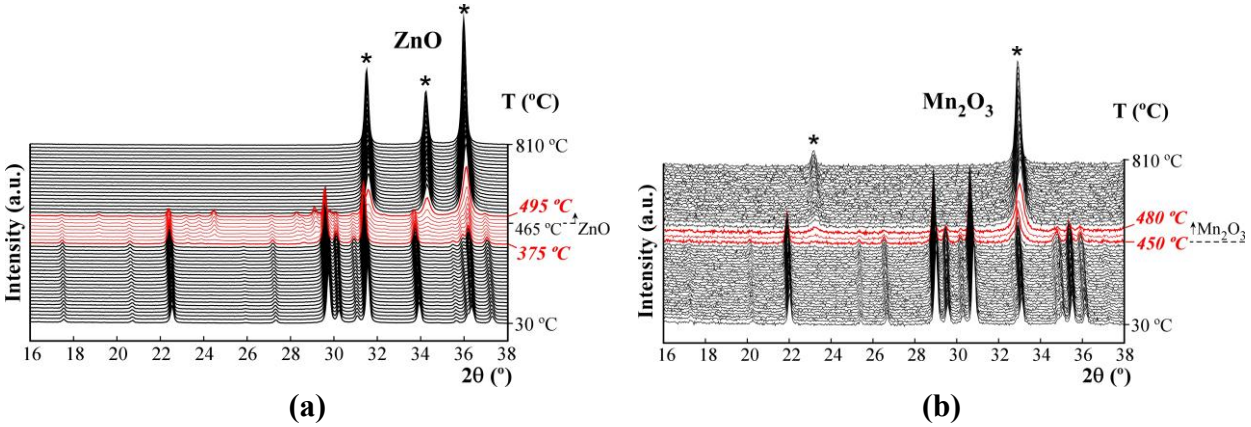


Figure S5. Thermodiffractograms of **(a)** $Zn_2(SeO_3)F_2$ (**1**) and **(b)** $Mn_2(SeO_3)F_2$ (**2**).

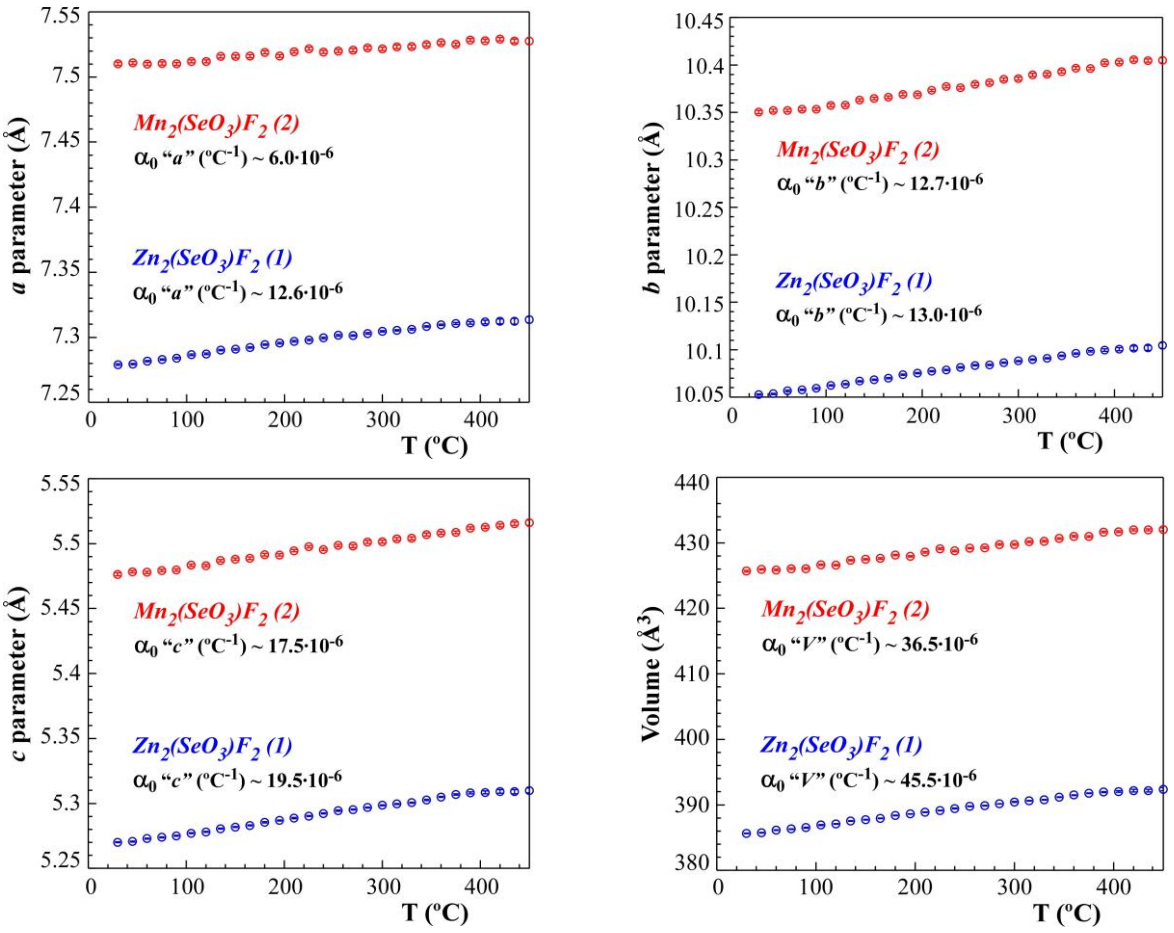


Figure S6. Thermal evolution of the parameters and volume of the unit cells for $Zn_2(SeO_3)F_2$ (**1**) and **(b)** $Mn_2(SeO_3)F_2$ (**2**) in the 30 to 450 ºC temperature range.

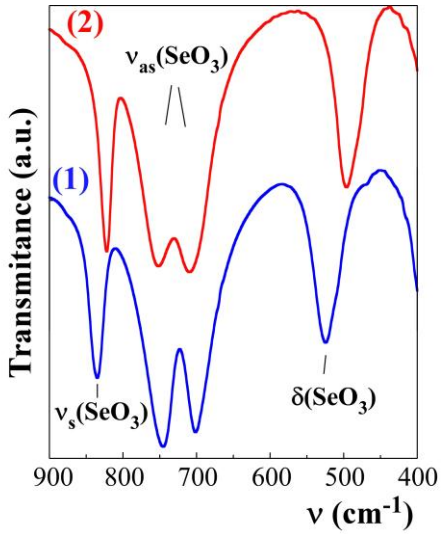


Figure S7. Infrared spectra of the compounds $Zn_2(SeO_3)F_2$ (**1**) and $Mn_2(SeO_3)F_2$ (**2**) in the 400 to 900 cm^{-1} frequency range.

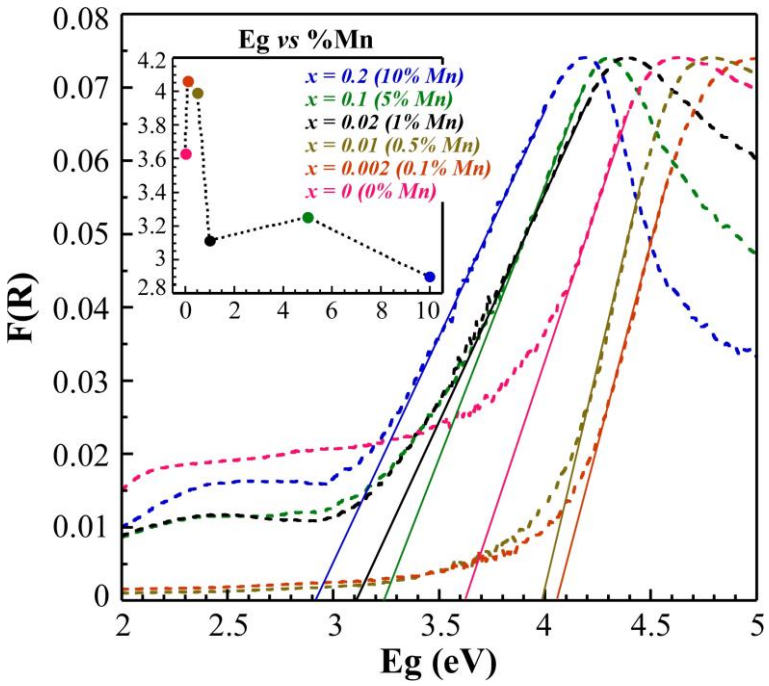


Figure S8. Diffuse reflectance spectra for $Zn_{2-x}Mn_x(SeO_3)F_2$ (x =0, 0.002, 0.01, 0.02, 0.1 and 0.2) compounds. Inset shows the variation in bandgap with Mn concentration.

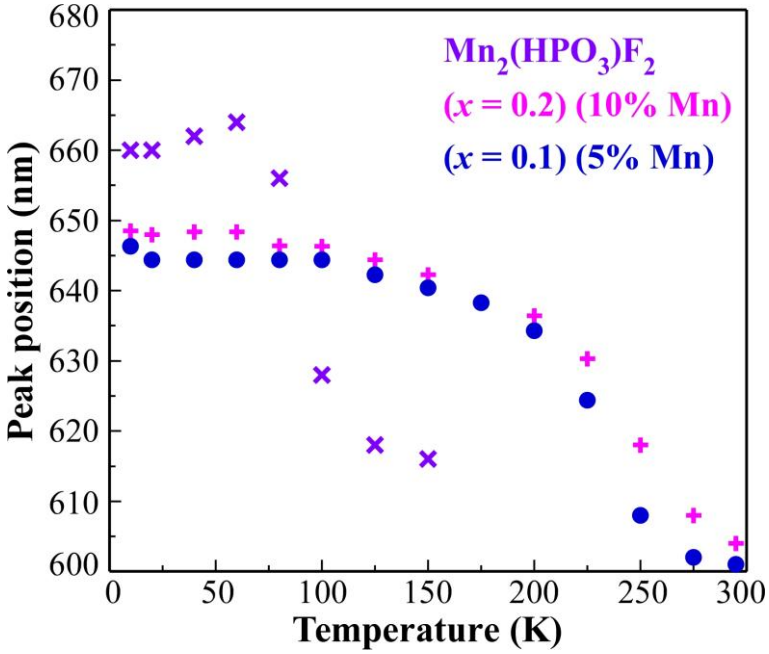


Figure S9. Peak position of the emission band as a function of temperature.

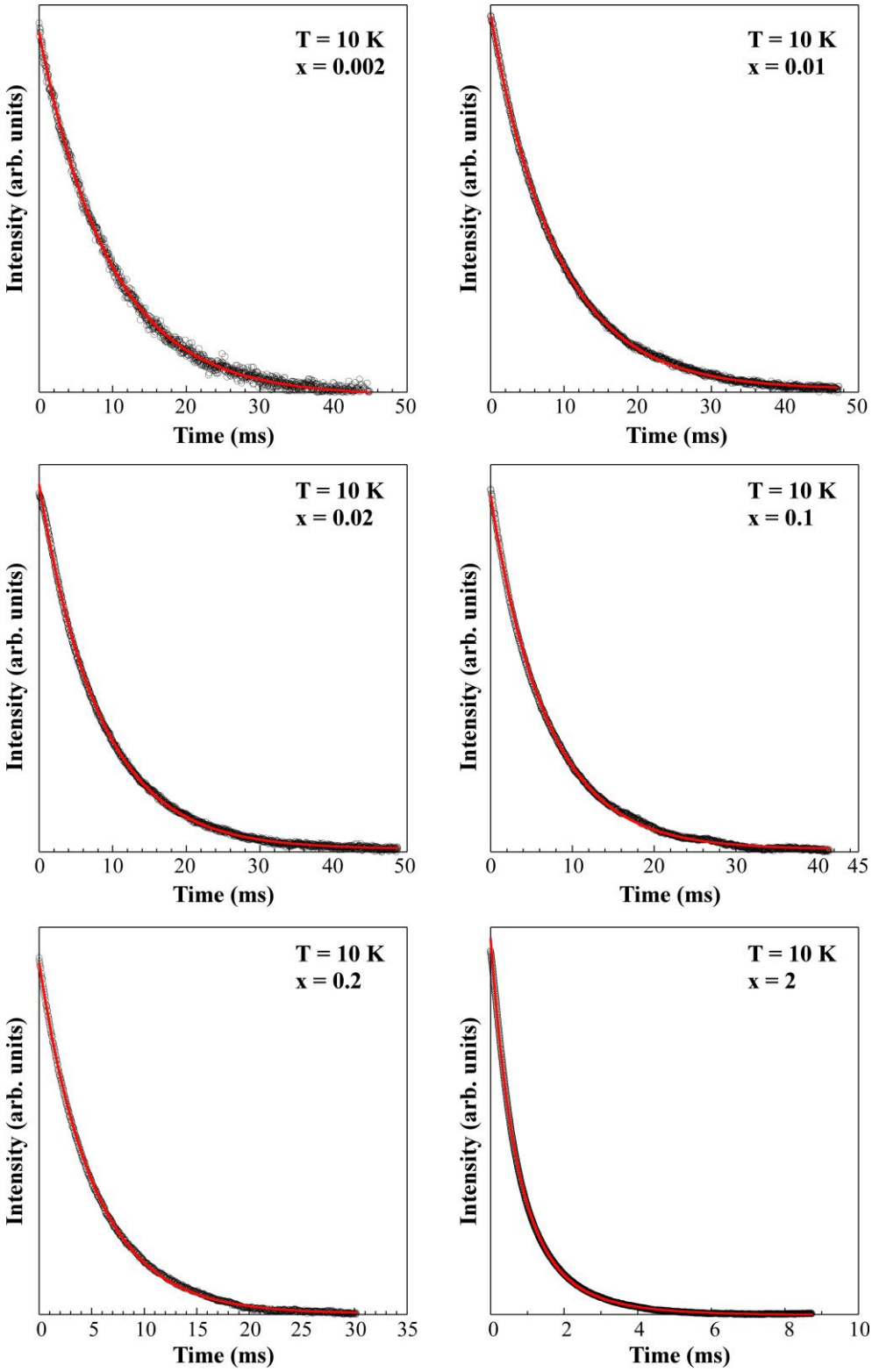
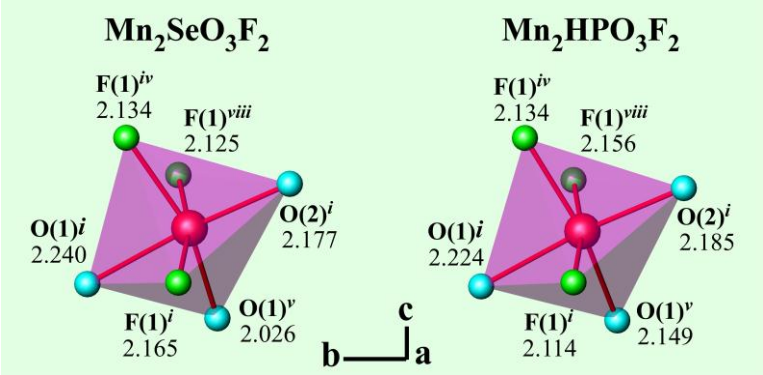


Figure S10. Experimental emission decay curves of the $^4T_1$ state for the samples $Zn_{2-x}Mn_x(SeO_3)F_2$ (x = 0.002, 0.01, 0.02, 0.1, 0.2, and 2) (symbols). The solid lines are the fits to an exponential function.



Atom	$Mn_2SeO_3F_2$	$Mn_2HPO_3F_2$
$O(1)^{v}$	**2.026**	**2.149**
$F(1)^{viii}$	2.125	2.156
$F(1)^{iv}$	2.134	2.134
$F(1)^{i}$	2.165	2.114
$O(2)^{i}$	2.177	2.185
$O(1)^{i}$	2.240	2.224
Δ (Mn-O,F)	2.026-2.240 ***(9.55%)***	2.114-2.224 **(4.95%)**

Figure S11. Ligand environment of manganese ion in $Mn_2(SeO_3)F_2$ (**2**) and $Mn_2(HPO_3)F_2$.

$Zn_2(SeO_3)F_2$ (1) – Rietveld Refinement

Table S1. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} ($Å^2$), for **(1)**.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} ($Å^2$)	*F. Oc.*
Zn(1)	*8d (1)*	0.09266(14)	0.43247(10)	0.2497(2)	1.85(2)	1.0
Se(1)	*4c (.m.)*	0.18035(18)	0.75000	0.1510(2)	1.89(3)	0.5
F(1)	*8d (1)*	0.3404(5)	0.4546(4)	0.0707(7)	1.95(10)	1.0
O(1)	*8d (1)*	0.0390(6)	0.6213(4)	0.0771(9)	1.85(12)	1.0
O(2)	*4c (.m.)*	0.1661(9)	0.25000	0.3956(12)	1.87(16)	0.5

Table S2. Bond distances (Å) and angles (°) for **(1)**.

$[Zn(1)O_3F_3]$

Zn(1)	**O(1)^{v}**	**F(1)^{i}**	**O(2)^{i}**	**F(1)^{viii}**	**F(1)^{iv}**	**O(1)^{i}**
O(1)^{i}	77.9(3)	82.5(3)	174.7(3)	86.4(3)	84.5(3)	***2.141(4)***
F(1)^{iv}	158.9(4)	96.2(3)	96.9(2)	77.3(2)	***2.095(4)***	
F(1)^{viii}	89.9(3)	167.6(3)	98.9(3)	***2.078(4)***		
O(2)^{i}	101.6(4)	92.3(3)	***2.059(3)***			
F(1)^{i}	93.1(3)	***2.047(4)***				
O(1)^{v}	***2.044(5)***					

$[Se(1)O_3]$

Se(1)	**O(1)^{i}**	**O(1)^{vii}**	**O(2)^{iv}**
O(2)^{iv}	102.2(5)	102.2(5)	***1.749(7)***
O(1)^{vii}	99.2(4)	***1.698(4)***	
O(1)^{i}	***1.698(4)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

$Zn_{1.998}Mn_{0.002}(SeO_3)F_2$ (x = 0.002) – Rietveld Refinement

Table S3. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} ($Å^2$), for ***x = 0.002***.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} ($Å^2$)	*F. Oc.*
Zn(1)	*8d (1)*	0.09244(16)	0.43234(12)	0.2496(3)	1.70(4)	0.99900
Mn(1)	*8d (1)*	0.09244(16)	0.43234(12)	0.2496(3)	1.70(4)	0.00100
Se(1)	*4c (.m.)*	0.1800(2)	0.75000	0.1507(3)	1.75(4)	0.50000
F(1)	*8d (1)*	0.3406(6)	0.4548(4)	0.0670(8)	1.99(12)	1.00000
O(1)	*8d (1)*	0.0425(7)	0.6208(5)	0.0778(11)	1.63(14)	1.00000
O(2)	*4c (.m.)*	0.1692(11)	0.25000	0.3938(14)	1.87(19)	0.50000

Table S4. Bond distances (Å) and angles (°) for ***x = 0.002***.

[(Zn,Mn)(1)O_3F_3]

Zn(1)/Mn(1)	**O(1)^{v}**	**F(1)^{i}**	**O(2)^{i}**	**F(1)^{iv}**	**F(1)^{viii}**	**O(1)^{i}**
O(1)^{i}	78.0(3)	81.6(3)	173.4(4)	84.1(3)	87.2(3)	***2.131(5)***
F(1)^{iv}	89.8(3)	167.5(4)	99.4(4)	76.9(3)	***2.085(5)***	
F(1)^{viii}	158.3(4)	96.3(3)	97.2(2)	***2.080(4)***		
O(2)^{i}	102.0(4)	91.8(3)	***2.062(4)***			
O(1)^{v}	93.2(3)	***2.060(5)***				
F(1)^{i}	***2.056(6)***					

[Se(1)O_3]

Se(1)	**O(1)^{i}**	**O(1)^{vii}**	**O(2)^{iv}**
O(1)^{i}	101.4(5)	101.4(5)	***1.743(8)***
O(1)^{vii}	100.9(4)	***1.684(5)***	
O(2)^{iv}	***1.684(5)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

$Zn_{1.99}Mn_{0.01}(SeO_3)F_2$ (x = 0.01) – Rietveld Refinement

Table S5. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} ($Å^2$), for ***x = 0.01***.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} ($Å^2$)	*F. Oc.*
Zn(1)	*8d (1)*	0.09289(17)	0.43278(12)	0.2493(3)	1.91(4)	0.99500
Mn(1)	*8d (1)*	0.09289(17)	0.43278(12)	0.2493(3)	1.91(4)	0.00500
Se(1)	*4c (.m.)*	0.1803(2)	0.75000	0.1514(3)	1.95(4)	0.50000
F(1)	*8d (1)*	0.3408(6)	0.4542(4)	0.0735(8)	1.92(11)	1.00000
O(1)	*8d (1)*	0.0399(7)	0.6203(5)	0.0763(11)	1.76(14)	1.00000
O(2)	*4c (.m.)*	0.1664(11)	0.25000	0.3970(15)	2.57(20)	0.50000

Table S6. Bond distances (Å) and angles (°) for ***x = 0.01***.

[(Zn,Mn)(1)O_3F_3]

Zn(1)/Mn(1)	**F(1)^{i}**	**O(1)^{v}**	**O(2)^{i}**	**F(1)^{viii}**	**F(1)^{iv}**	**O(1)^{i}**
O(1)^{i}	82.7(3)	77.6(3)	174.6(4)	86.6(3)	84.9(3)	***2.130(5)***
F(1)^{iv}	96.2(3)	158.6(4)	96.6(3)	77.4(3)	***2.108(4)***	
F(1)^{viii}	168.0(4)	89.2(3)	98.8(4)	***2.071(5)***		
O(2)^{i}	92.1(3)	101.9(4)	***2.067(4)***			
O(1)^{v}	93.7(3)	***2.041(6)***				
F(1)^{i}	***2.040(5)***					

[Se(1)O_3]

Se(1)	**O(1)^{i}**	**O(1)^{vii}**	**O(2)^{iv}**
O(1)^{i}	101.8(5)	101.8(5)	***1.745(8)***
O(1)^{vii}	99.9(4)	***1.704(5)***	
O(2)^{iv}	***1.704(5)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

$Zn_{1.98}Mn_{0.02}(SeO_3)F_2$ (x = 0.02) – Rietveld Refinement

Table S7. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} ($Å^2$), for ***x = 0.02***.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} ($Å^2$)	*F. Oc.*
Zn(1)	*8d (1)*	0.09287(17)	0.43258(13)	0.2501(3)	1.47(3)	0.99000
Mn(1)	*8d (1)*	0.09287(17)	0.43258(13)	0.2501(3)	1.47(3)	0.01000
Se(1)	*4c (.m.)*	0.1803(2)	0.75000	0.1510(3)	1.67(4)	0.50000
F(1)	*8d (1)*	0.3413(6)	0.4557(4)	0.0709(8)	1.55(11)	1.00000
O(1)	*8d (1)*	0.0375(7)	0.6201(5)	0.0782(11)	1.25(14)	1.00000
O(2)	*4c (.m.)*	0.1698(12)	0.25000	0.3965(15)	2.3(2)	0.50000

Table S8. Bond distances (Å) and angles (°) for ***x = 0.02***.

[(Zn,Mn)(1)O_3F_3]

Zn(1)/Mn(1)	**O(1)^{v}**	**F(1)^{i}**	**O(2)^{i}**	**F(1)^{viii}**	**F(1)^{iv}**	**O(1)^{i}**
O(1)^{i}	77.4(3)	82.6(3)	174.4(4)	85.8(3)	84.9(3)	***2.131(5)***
F(1)^{iv}	158.9(4)	96.3(3)	96.5(3)	76.9(3)	***2.086(4)***	
F(1)^{viii}	90.2(3)	167.1(4)	99.7(4)	***2.074(5)***		
O(2)^{i}	102.2(4)	91.9(3)	***2.069(4)***			
F(1)^{i}	92.8(3)	***2.054(5)***				
O(1)^{v}	***2.044(6)***					

[Se(1)O_3]

Se(1)	**O(1)^{i}**	**O(1)^{vii}**	**O(2)^{iv}**
O(1)^{i}	102.1(6)	102.1(6)	***1.730(8)***
O(1)^{vii}	99.4(4)	***1.713(5)***	
O(2)^{iv}	***1.713(5)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

$Zn_{1.9}Mn_{0.1}(SeO_3)F_2$ (x = 0.1) – Rietveld Refinement

Table S9. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} ($Å^2$), for ***x = 0.1***.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} ($Å^2$)	*F. Oc.*
Zn(1)	*8d (1)*	0.09302(16)	0.43263(12)	0.2508(3)	1.85(4)	0.95000
Mn(1)	*8d (1)*	0.09302(16)	0.43263(12)	0.2508(3)	1.85(4)	0.05000
Se(1)	*4c (.m.)*	0.1801(2)	0.75000	0.1506(2)	2.01(4)	0.50000
F(1)	*8d (1)*	0.3411(6)	0.4536(4)	0.0725(8)	1.94(11)	1.00000
O(1)	*8d (1)*	0.0367(7)	0.6197(4)	0.0739(10)	1.79(14)	1.00000
O(2)	*4c (.m.)*	0.1705(11)	0.25000	0.3998(14)	2.07(19)	0.50000

Table S10. Bond distances (Å) and angles (°) for ***x = 0.1***.

[(Zn,Mn)(1)O_3F_3]

Zn(1)/Mn(1)	**O(1)^{v}**	**F(1)^{i}**	**F(1)^{viii}**	**O(2)^{i}**	**F(1)^{iv}**	**O(1)^{i}**
O(1)^{i}	76.7(3)	83.0(3)	86.4(3)	174.3(3)	85.2(3)	***2.143(5)***
F(1)^{iv}	158.5(4)	96.5(3)	77.5(3)	96.5(2)	***2.105(4)***	
O(2)^{i}	102.5(4)	91.4(3)	99.2(4)	***2.079(4)***		
F(1)^{viii}	89.6(3)	168.2(4)	***2.071(5)***			
F(1)^{i}	92.9(3)	***2.050(5)***				
O(1)^{v}	***2.028(5)***					

[Se(1)O_3]

Se(1)	**O(2)^{iv}**	**O(1)^{i}**	**O(1)^{vii}**
O(1)^{i}	101.7(5)	99.0(4)	***1.726(5)***
O(1)^{i}	101.7(5)	***1.726(5)***	
O(2)^{iv}	***1.715(8)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

$Zn_{1.8}Mn_{0.2}(SeO_3)F_2$ (x = 0.2) – Rietveld Refinement

Table S11. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} ($Å^2$), for ***x = 0.2***.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} ($Å^2$)	*F. Oc.*
Zn(1)	*8d (1)*	0.09265(17)	0.43253(13)	0.2508(3)	1.69(4)	0.90000
Mn(1)	*8d (1)*	0.09265(17)	0.43253(13)	0.2508(3)	1.69(4)	0.10000
Se(1)	*4c (.m.)*	0.1795(2)	0.75000	0.1510(3)	1.88(4)	0.50000
F(1)	*8d (1)*	0.3423(6)	0.4539(4)	0.0734(8)	1.80(12)	1.00000
O(1)	*8d (1)*	0.0368(8)	0.6209(5)	0.0742(11)	1.90(15)	1.00000
O(2)	*4c (.m.)*	0.1700(11)	0.25000	0.4004(14)	2.09(20)	0.50000

Table S12. Bond distances (Å) and angles (°) for ***x = 0.2***.

[(Zn,Mn)(1)O_3F_3]

Zn(1)/Mn(1)	**O(1)^{v}**	**F(1)^{i}**	**F(1)^{viii}**	**O(2)^{i}**	**F(1)^{iv}**	**O(1)^{i}**
O(1)^{i}	77.2(3)	83.0(3)	86.3(3)	174.4(4)	85.1(3)	***2.157(5)***
F(1)^{iv}	158.8(4)	96.5(3)	77.2(3)	96.4(2)	***2.110(4)***	
O(2)^{i}	102.3(4)	91.5(3)	99.3(4)	***2.083(4)***		
F(1)^{viii}	89.8(4)	168.0(4)	***2.063(5)***			
F(1)^{i}	93.1(4)	***2.062(5)***				
O(1)^{v}	***2.035(6)***					

[Se(1)O_3]

Se(1)	**O(1)^{i}**	**O(1)^{vii}**	**O(2)^{iv}**
O(2)^{iv}	101.8(6)	101.8(6)	***1.723(8)***
O(1)^{vii}	98.7(4)	***1.717(5)***	
O(1)^{i}	***1.717(5)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

$Mn_2(SeO_3)F_2$ (2) – Rietveld Refinement

Table S13. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} ($Å^2$), for **(2)**.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} ($Å^2$)	*F. Oc.*
Mn(1)	*8d (1)*	0.0935(4)	0.4323(2)	0.2519(5)	1.47(7)	1.00000
Se(1)	*4c (.m.)*	0.1759(4)	0.75000	0.1498(4)	1.68(7)	0.50000
F(1)	*8d (1)*	0.3458(10)	0.4527(7)	0.0644(11)	1.30(17)	1.00000
O(1)	*8d (1)*	0.0348(12)	0.6183(8)	0.0591(16)	2.1(3)	1.00000
O(2)	*4c (.m.)*	0.1853(18)	0.25000	0.405(2)	2.0(3)	0.50000

Table S14. Bond distances (Å) and angles (°) for **(2)**.

$[Mn(1)O_3F_3]$

Mn(1)	**O(1)^{v}**	**F(1)^{viii}**	**F(1)^{iv}**	**F(1)^{i}**	**O(2)^{i}**	**O(1)^{i}**
O(1)^{i}	74.5(5)	88.0(5)	86.6(5)	82.2(5)	171.5(6)	***2.240(9)***
O(2)^{i}	104.5(7)	100.4(6)	96.1(4)	89.4(5)	***2.177(6)***	
F(1)^{i}	92.4(6)	168.7(6)	98.0(5)	***2.165(8)***		
F(1)^{iv}	156.9(7)	75.6(4)	***2.134(7)***			
F(1)^{viii}	90.4(5)	***2.125(8)***				
O(1)^{v}	***2.026(9)***					

$[Se(1)O_3]$

Se(1)	**O(2)^{iv}**	**O(1)^{i}**	**O(1)^{vii}**
O(1)^{vii}	98.3(9)	98.7(7)	***1.796(9)***
O(1)^{i}	98.3(9)	***1.796(9)***	
O(2)^{iv}	***1.698(12)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

$Zn_2(SeO_3)F_2$ (1) and $Mn_2(SeO_3)F_2$ (2)
Rietveld Refinement (Structural model of $Co_2(SeO_3)F_2$)

Table S15. Crystallographic data and structure Rietveld refinement parameters for (**1**) and (**2**) from the structural model of $Co_2(SeO_3)F_2$.

Phase	**$Zn_2(SeO_3)F_2$ (1)**	**$Mn_2(SeO_3)F_2$ (2)**
a, Å	7.27928(5)	7.5086(11)
b, Å	10.05272(7)	10.3502(14)
c, Å	5.26967(4)	5.47702(7)
V, Å^3	385.617(5)	425.651(10)
Independent Reflections	239	264
Structural Parameters	18	18
Profile Parameters	53	46
Soft Distance Constraints	0	0
R_{Bragg}	3.48	13.4
R_f	1.99	8.79
R_p	10.0	21.4
R_{wp}	12.8	26.0
R_{exp}	9.44	17.14
χ^2	*1.84*	*2.31*

Table S16. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} (Å^2), for **(1)**.

Atoms	***Wyckoff***	***X***	***Y***	***Z***	***B_{iso} (Å^2)***	***F. Oc.***
Se(1)	*4c (.m.)*	0.68034(19)	0.25000	0.1510(2)	1.88(4)	0.50000
Zn(1)	*8d (1)*	0.59264(15)	0.56755(11)	0.2496(3)	1.84(4)	1.00000
F(1)	*8d (1)*	0.6596(6)	0.4545(4)	0.5707(7)	1.92(11)	1.00000
O(1)	*4c (.m.)*	0.6659(10)	0.75000	0.3954(13)	1.87(17)	0.50000
O(2)	*8d (1)*	0.5390(7)	0.3786(4)	0.0770(10)	1.84(14)	1.00000

Table S17. Bond distances (Å) and angles (°) for **(1)**.

[$Zn(1)O_3F_3$]

Zn(1)	**O(2)^v**	**F(1)^{iv}**	**O(1)^i**	**F(1)^v**	**F(1)^i**	**O(2)^i**
O(2)^i	78.0(3)	82.5(3)	174.7(3)	86.4(3)	84.5(3)	***2.142(4)***
F(1)^i	158.9(4)	96.2(3)	97.0(2)	77.3(3)	***2.096(4)***	
F(1)^v	89.9(3)	167.7(4)	98.9(3)	***2.078(4)***		
O(1)^i	101.5(4)	92.3(3)	***2.059(3)***			
F(1)^{iv}	93.1(3)	***2.047(4)***				
O(2)^v	***2.043(5)***					

[Se(1)O$_3$]

Se(1)	O(2)^{i}	O(2)^{vii}	O(1)^{iv}
O(1)^{iv}	102.2(5)	102.2(5)	***1.751(7)***
O(2)^{vii}	99.2(4)	***1.698(5)***	
O(2)^{i}	***1.698(5)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.

Table S18. Atomic coordinates and equivalent isotropic displacement parameters, B_{iso} (Å^2), for **(2)**.

Atoms	*Wyckoff*	*X*	*Y*	*Z*	B_{iso} (Å^2)	*F. Oc.*
Se(1)	*4c (.m.)*	0.6757(4)	0.25000	0.1497(4)	1.88(6)	0.50000
Mn(1)	*8d (1)*	0.5935(4)	0.5677(2)	0.2519(5)	1.68(6)	1.00000
F(1)	*8d (1)*	0.6543(10)	0.4526(7)	0.5645(11)	1.59(18)	1.00000
O(1)	*4c (.m.)*	0.6845(18)	0.75000	0.406(2)	2.1(3)	0.50000
O(2)	*8d (1)*	0.5347(13)	0.3816(9)	0.0587(17)	2.5(3)	1.00000

Table S19. Bond distances (Å) and angles (°) for **(2)**.

[Mn(1)O$_3$F$_3$]

Mn(1)	O(2)^{v}	F(1)^{v}	F(1)^{i}	F(1)^{iv}	O(1)^{i}	O(2)^{i}
O(2)^{i}	74.5(6)	88.0(5)	86.6(5)	82.2(5)	171.7(6)	***2.242(10)***
O(1)^{i}	104.5(7)	100.2(6)	96.1(4)	89.6(5)	***2.177(6)***	
F(1)^{iv}	92.4(6)	168.8(6)	98.0(5)	***2.164(8)***		
F(1)^{i}	157.0(7)	75.7(4)	***2.135(7)***			
F(1)^{v}	90.4(6)	***2.125(8)***				
O(2)^{v}	***2.024(10)***					

[Se(1)O$_3$]

Se(1)	O(1)^{iv}	O(2)^{i}	O(2)^{vii}
O(2)^{vii}	98.4(9)	98.7(8)	***1.796(10)***
O(2)^{i}	98.4(9)	***1.796(10)***	
O(1)^{iv}	***1.698(12)***		

Symmetry codes: *i* = x, y, z; *ii* = x+1/2, -y+1/2, -z+1/2; *iii* = -x, y+1/2, -z; *iv* = -x+1/2, -y, z+1/2; *v* = -x, -y, -z; *vi* = -x+1/2, y+1/2, z+1/2; *vii* = x, -y+1/2, z; *viii* = x+1/2, y, -z+1/2.