Crystal-to-Crystal Transformation of a New Selenite Compound $CaNi_2(SeO_3)_3 \cdot 2H_2O$ Induced by a Dehydration

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Fig. S1. Simulated and experimental powder X-ray (Cu Ka) diffraction (XRD) patterns for (a) $CaNi_2(SeO_3)_3 \cdot 2H_2O$, (b) $CaNi_2(SeO_3)_3 \cdot 1.5H_2O$ and (c) $CaNi_2(SeO_3)_3$ and $CaNi_2(SeO_3)_3 \cdot 2H_2O$ annealed at 500 ℃.

Fig. S2. The powder XRD patterns of **2** in water heated at different temperatures, respectively.

Fig. S3. The magnetic susceptibility of **3** measured at 0.1 T with heating and cooling regimes.

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters for $CaNi_2(SeO_3)_3 \cdot 2H_2O$.

Table S2. Anisotropic displacement parameters for $CaNi_2(SeO_3)_3 \cdot 2H_2O$.

Table S3. Selected bond lengths and bond angles of $CaNi_2(SeO_3)_3 \cdot 2H_2O$.

Table S4. Fractional atomic coordinates and equivalent isotropic displacement parameters for $CaNi_2(SeO_3)_3 \cdot 1.5H_2O$.

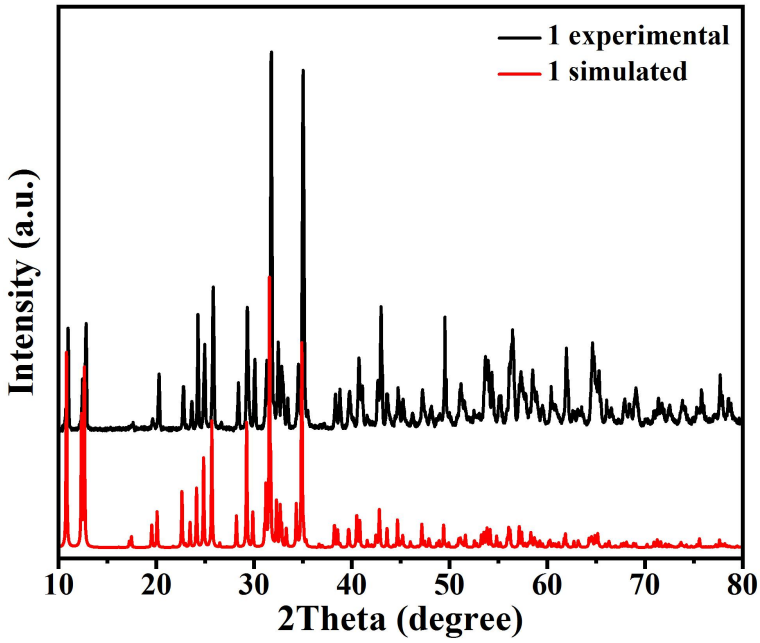
Table S5. Anisotropic displacement parameters for $CaNi_2(SeO_3)_3 \cdot 1.5H_2O$.

Table S6. Selected bond lengths and bond angles of $CaNi_2(SeO_3)_3 \cdot 1.5H_2O$.

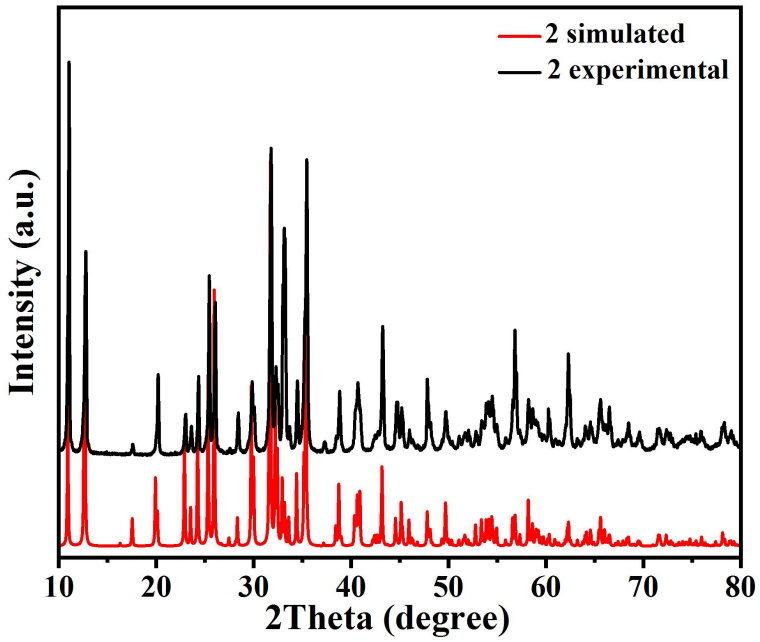
Table S7. Fractional atomic coordinates and equivalent isotropic displacement parameters for $CaNi_2(SeO_3)_3$.

Table S8. Anisotropic displacement parameters for $CaNi_2(SeO_3)_3$.

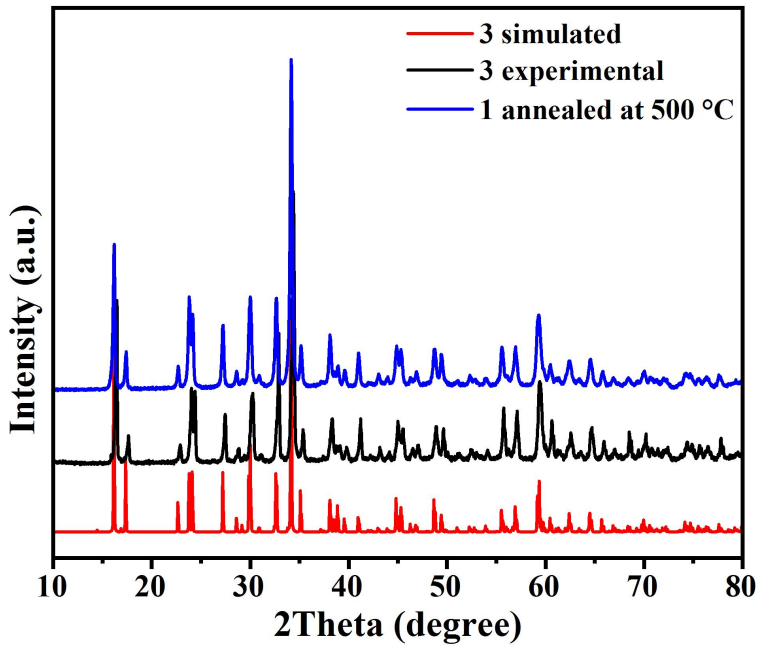
Table S9. Selected bond lengths and bond angles of $CaNi_2(SeO_3)_3$.


1 experimental
1 simulated
Intensity (a.u.)
10
20
30
40
50
60
70
80
2Theta (degree)

(a)


2 simulated
2 experimental
Intensity (a.u.)
10
20
30
40
50
60
70
80
2Theta (degree)

(b)



(c)

Fig. S1. Simulated and experimental powder X-ray (Cu Ka) diffraction patterns for (a) **1**, (b) **2** and (c) **3** and **1** annealed at 500 ℃.

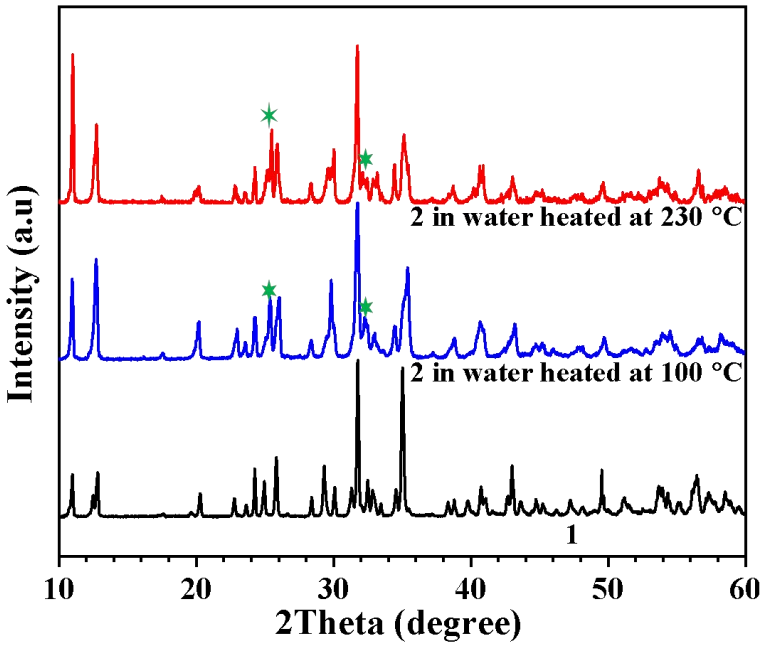


Fig. S2. The powder X-ray (Cu Ka) diffraction patterns of **2** in water heated at 100 ℃ for 2 days and 230 ℃ for 1 day, showing the differences (star-marked) between **2** heated and **1**.

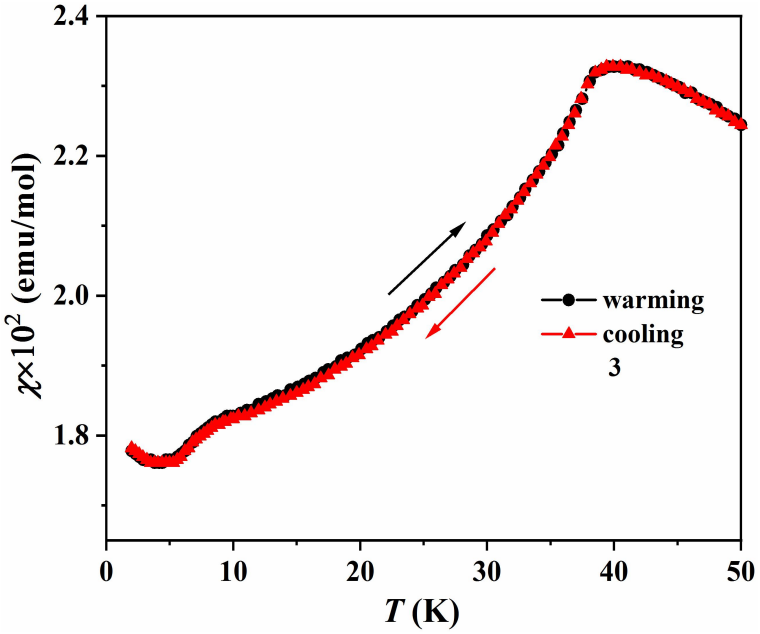


Fig. S3. The magnetic susceptibility of **3** measured at 0.1 T with warming and cooling regimes.

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $CaNi_2(SeO_3)_3 \cdot 2H_2O$. U_{eq} is defined as one third of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ni1	1797.5(7)	5584.5(7)	3161.1(6)	8.93(12)
Se1	67.2(7)	2500	415.4(7)	8.57(12)
Se2	304.8(7)	2500	4804.5(7)	9.30(12)
Se3	5331.7(7)	2500	3277.3(7)	8.41(12)
O1	-364(4)	4251(4)	1436(4)	13.0(6)
O2	-1935(5)	2500	-1401(5)	9.1(7)
O3	1895(4)	4219(4)	5170(4)	12.9(6)
O4	65(6)	2500	6623(5)	10.1(8)
O5	3930(4)	4331(4)	2798(4)	13.0(6)
O6	6197(5)	2500	5395(5)	11.4(8)
Ca1	4617.6(16)	2500	7129.6(16)	15.2(2)
O1W	3616(6)	4291(7)	8918(6)	38.5(14)
O1B	3820(60)	2500	9170(40)	87(14)
H(1WA)	3930(20)	3980(30)	9882(14)	58
H(1WB)	2640(60)	4890(80)	8550(30)	58
H(1BA)	2687	2500	8656	131
H(1BB)	4201	2301	10157	131

Table S2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $CaNi_2(SeO_3)_3 \cdot 2H_2O$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	10.2(2)	6.3(2)	11.0(3)	-0.15(19)	4.96(19)	-0.57(18)
Se1	8.3(2)	7.8(3)	9.5(3)	0	3.6(2)	0
Se2	9.9(2)	7.9(3)	11.7(3)	0	6.1(2)	0
Se3	8.3(2)	7.0(3)	10.4(3)	0	4.3(2)	0
O1	14.2(13)	10.4(15)	15.7(16)	-4.0(11)	7.3(12)	-2.0(11)
O2	8.9(17)	8.1(19)	7.7(18)	0	0.5(14)	0
O3	12.7(13)	10.9(15)	16.2(15)	4.3(11)	7.1(12)	-1.1(11)
O4	17.0(19)	2.6(18)	14(2)	0	9.3(17)	0
O5	13.4(13)	10.0(15)	15.2(15)	4.0(11)	5.6(12)	5.7(11)
O6	13.0(18)	11(2)	8.8(19)	0	3.2(16)	0
Ca1	12.3(5)	15.6(6)	17.1(6)	0	5.4(5)	0
O1W	40(3)	47(4)	35(3)	3(2)	23(2)	13(2)
O1B	100(20)	90(30)	43(19)	0	0(18)	0

Table S3. Selected bond lengths (Å) and bond angles (°) of $CaNi_2(SeO_3)_3 \cdot 2H_2O$.

Bond	Dist.	Bond	Dist.
Ni(1)-O(1)	2.021(3)	Se(2)-O(4)	1.717(4)
Ni(1)-O(2)#1	2.154(3)	Se(3)-O(5)#4	1.682(3)
Ni(1)-O(3)	2.038(3)	Se(3)-O(5)	1.682(3)
Ni(1)-O(4)#2	2.099(3)	Se(3)-O(6)	1.735(4)
Ni(1)-O(5)	2.053(3)	O(2)-Ca(1)#5	2.477(4)
Ni(1)-O(6)#3	2.116(3)	O(3)-Ca(1)	2.486(3)
Se(1)-O(1)#4	1.695(3)	O(5)-Ca(1)#3	2.590(3)
Se(1)-O(1)	1.695(3)	O(6)-Ca(1)	2.355(4)
Se(1)-O(2)	1.738(4)	Ca(1)-O(1W)#4	2.445(4)
Se(2)-O(3)	1.714(3)	Ca(1)-O(1W)	2.445(4)
Se(2)-O(3)#4	1.714(3)	Ca(1)-O(1B)	2.17(4)
Angle	(°)	Angle	(°)
O(1)-Ni(1)-O(2)#1	92.14(12)	O(3)#4-Ca(1)-O(3)	61.30(13)
O(1)-Ni(1)-O(3)	98.68(12)	O(3)-Ca(1)-O(5)#3	78.46(9)
O(1)-Ni(1)-O(4)#2	90.00(13)	O(3)#4-Ca(1)-O(5)#8	78.46(9)
O(1)-Ni(1)-O(5)	98.22(11)	O(3)-Ca(1)-O(5)#8	136.05(11)
O(1)-Ni(1)-O(6)#3	166.73(12)	O(3)#4-Ca(1)-O(5)#3	136.05(11)
O(3)-Ni(1)-O(2)#1	167.72(12)	O(5)#3-Ca(1)-O(5)#8	128.95(13)
O(3)-Ni(1)-O(4)#2	91.43(12)	O(6)-Ca(1)-O(2)#9	66.03(14)
O(3)-Ni(1)-O(5)	100.45(12)	O(6)-Ca(1)-O(3)#4	93.84(11)
O(3)-Ni(1)-O(6)#3	92.34(13)	O(6)-Ca(1)-O(3)	93.84(11)
O(4)#2-Ni(1)-O(2)#1	82.72(12)	O(6)-Ca(1)-O(5)#8	70.74(7)
O(4)#2-Ni(1)-O(6)#3	82.32(13)	O(6)-Ca(1)-O(5)#3	70.74(7)
O(5)-Ni(1)-O(2)#1	83.63(12)	O(6)-Ca(1)-O(1W)#4	146.38(12)

O(5)-Ni(1)-O(4)#2	164.30(11)	O(6)-Ca(1)-O(1W)	146.38(12)
O(5)-Ni(1)-O(6)#3	86.94(12)	O(1W)#4-Ca(1)-O(2)#9	103.15(14)
O(6)#3-Ni(1)-O(2)#1	76.22(13)	O(1W)-Ca(1)-O(2)#9	103.15(14)
O(1)-Se(1)-O(1)#4	99.21(19)	O(1W)#4-Ca(1)-O(3)	108.88(14)
O(1)-Se(1)-O(2)	101.62(13)	O(1W)-Ca(1)-O(3)#4	108.88(14)
O(1)#4-Se(1)-O(2)	101.62(13)	O(1W)#4-Ca(1)-O(3)#4	76.87(14)
O(3)#4-Se(2)-O(3)	95.37(19)	O(1W)-Ca(1)-O(3)	76.87(13)
O(3)#4-Se(2)-O(4)	100.03(14)	O(1W)#4-Ca(1)-O(5)#3	136.77(14)
O(3)-Se(2)-O(4)	100.03(14)	O(1W)-Ca(1)-O(5)#3	75.73(14)
O(5)#4-Se(3)-O(5)	106.7(2)	O(1W)-Ca(1)-O(5)#8	136.76(14)
O(5)#4-Se(3)-O(6)	101.56(13)	O(1W)#4-Ca(1)-O(5)#8	75.73(14)
O(5)-Se(3)-O(6)	101.56(13)	O(1W)-Ca(1)-O(1W)#4	65.4(2)
O(2)#9-Ca(1)-O(3)#4	144.19(8)	O(1B)-Ca(1)-O(3)	97.8(9)
O(2)#9-Ca(1)-O(3)	144.19(8)	O(1B)-Ca(1)-O(6)	166.5(10)
O(2)#9-Ca(1)-O(5)#3	67.21(7)	O(1B)-Ca(1)-O(1W)#4	33.07(19)
O(2)#9-Ca(1)-O(5)#8	67.21(7)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z; #2 -x,-y+1,-z+1; #3 -x+1,-y+1,-z+1; #4 x,-y+1/2,z; #5 x-1,y,z-1; #6 -x,y-1/2,-z; #7 -x,y-1/2,-z+1; #8 -x+1,y-1/2,-z+1; #9 x+1,y,z+1.

Table S4. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $CaNi_2(SeO_3)_3 \cdot 1.5H_2O$. U_{eq} is defined as one third of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ni(1)	1757(1)	5584(1)	3137(1)	8(1)
Se(1)	57(1)	2500	463(1)	8(1)
Se(2)	317(1)	2500	4812(1)	8(1)
Se(3)	5362(1)	2500	3255(1)	7(1)
O(1)	-462(3)	4269(3)	1415(2)	13(1)
O(2)	-1920(4)	2500	-1431(3)	9(1)
O(3)	1934(3)	4230(3)	5192(2)	11(1)
O(4)	144(4)	2500	6658(3)	10(1)
O(5)	3935(3)	4343(3)	2743(3)	13(1)
O(6)	6194(4)	2500	5379(3)	11(1)
Ca(1)	4693(1)	2500	7153(1)	14(1)
O(1W)	4060(20)	4150(30)	9263(15)	125(7)
O(1B)	3676(18)	2500	9217(16)	97(8)
H(1WA)	4410(70)	3700(50)	10190(30)	187
H(1WB)	3100(200)	4800(300)	8970(60)	187
H(1BA)	2539	2500	8698	146
H(1BB)	4053	2301	10199	146

Table S5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $CaNi_2(SeO_3)_3 \cdot 1.5H_2O$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Ni(1)	9(1)	8(1)	6(1)	0(1)	3(1)	-1(1)
Se(1)	7(1)	10(1)	6(1)	0	1(1)	0
Se(2)	6(1)	9(1)	7(1)	0	3(1)	0
Se(3)	6(1)	9(1)	7(1)	0	2(1)	0
O(1)	12(1)	14(1)	11(1)	-6(1)	4(1)	-2(1)
O(2)	8(1)	11(1)	5(1)	0	-1(1)	0
O(3)	10(1)	12(1)	10(1)	1(1)	4(1)	-3(1)
O(4)	13(1)	11(1)	9(1)	0	7(1)	0
O(5)	11(1)	11(1)	14(1)	3(1)	4(1)	4(1)
O(6)	11(1)	12(1)	6(1)	0	0(1)	0
Ca(1)	9(1)	17(1)	15(1)	0	3(1)	0
O(1W)	119(11)	220(20)	61(7)	-42(10)	59(7)	-52(12)
O(1B)	27(5)	240(30)	29(6)	0	14(4)	0

Table S6. Selected bond lengths (Å) and bond angles (°) of $CaNi_2(SeO_3)_3 \cdot 1.5H_2O$.

Bond	Dist.	Bond	Dist.
Ni(1)-O(1)	2.003(2)	Se(2)-O(4)	1.712(3)
Ni(1)-O(2)#1	2.116(2)	Se(3)-O(5)	1.6829(19)
Ni(1)-O(3)	2.0407(19)	Se(3)-O(5)#4	1.6830(19)
Ni(1)-O(4)#2	2.101(2)	Se(3)-O(6)	1.726(3)
Ni(1)-O(5)	2.077(2)	O(2)-Ca(1)#5	2.385(3)
Ni(1)-O(6)#3	2.115(2)	O(3)-Ca(1)	2.466(2)
Se(1)-O(1)#4	1.691(2)	O(5)-Ca(1)#3	2.534(2)
Se(1)-O(1)	1.691(2)	O(6)-Ca(1)	2.333(3)
Se(1)-O(2)	1.737(3)	Ca(1)-O(1W)#4	2.458(13)
Se(2)-O(3)	1.7142(19)	Ca(1)-O(1W)	2.458(13)
Angle	(°)	Angle	(°)
O(1)-Ni(1)-O(2)#1	93.48(9)	O(2)#9-Ca(1)-O(1W)#4	97.3(3)
O(1)-Ni(1)-O(3)	99.51(8)	O(2)#9-Ca(1)-O(1W)	97.3(4)
O(1)-Ni(1)-O(4)#2	89.02(9)	O(3)-Ca(1)-O(3)#4	61.94(9)
O(1)-Ni(1)-O(5)	98.90(8)	O(3)-Ca(1)-O(5)#3	77.33(6)
O(1)-Ni(1)-O(6)#3	166.89(8)	O(3)-Ca(1)-O(5)#8	136.14(7)
O(3)-Ni(1)-O(2)#1	165.85(8)	O(3)#4-Ca(1)-O(5)#3	136.14(7)
O(3)-Ni(1)-O(4)#2	91.61(9)	O(3)#4-Ca(1)-O(5)#8	77.32(6)
O(3)-Ni(1)-O(5)	101.01(8)	O(5)#3-Ca(1)-O(5)#8	132.08(10)
O(3)-Ni(1)-O(6)#3	90.74(9)	O(6)-Ca(1)-O(2)#9	66.71(9)
O(4)#2-Ni(1)-O(2)#1	82.97(9)	O(6)-Ca(1)-O(3)#4	92.89(8)
O(4)#2-Ni(1)-O(6)#3	82.50(9)	O(6)-Ca(1)-O(3)	92.89(8)
O(5)-Ni(1)-O(2)#1	82.35(9)	O(6)-Ca(1)-O(5)#3	72.64(6)
O(5)-Ni(1)-O(4)#2	163.70(8)	O(6)-Ca(1)-O(5)#8	72.64(6)
O(5)-Ni(1)-O(6)#3	87.03(9)	O(6)-Ca(1)-O(1W)	147.3(4)

O(6)#3-Ni(1)-O(2)#1	75.63(9)	O(6)-Ca(1)-O(1W)#4	147.3(4)
O(1)#4-Se(1)-O(1)	100.19(15)	O(1W)#4-Ca(1)-O(3)	113.7(3)
O(1)-Se(1)-O(2)	100.97(9)	O(1W)-Ca(1)-O(3)	84.1(4)
O(1)#4-Se(1)-O(2)	100.97(9)	O(1W)#4-Ca(1)-O(3)#4	84.1(4)
O(3)-Se(2)-O(3)#4	95.51(13)	O(1W)-Ca(1)-O(3)#4	113.7(4)
O(4)-Se(2)-O(3)	99.16(9)	O(1W)#4-Ca(1)-O(5)#3	129.7(5)
O(4)-Se(2)-O(3)#4	99.16(9)	O(1W)-Ca(1)-O(5)#3	74.9(4)
O(5)-Se(3)-O(5)#4	106.86(14)	O(1W)#4-Ca(1)-O(5)#8	74.9(4)
O(5)-Se(3)-O(6)	101.26(9)	O(1W)-Ca(1)-O(5)#8	129.7(5)
O(5)#4-Se(3)-O(6)	101.27(9)	O(1W)#4-Ca(1)-O(1W)	58.9(9)
O(2)#9-Ca(1)-O(3)#4	143.72(6)	O(1B)-Ca(1)-O(3)	94.6(3)
O(2)#9-Ca(1)-O(3)	143.72(6)	O(1B)-Ca(1)-O(6)	171.3(3)
O(2)#9-Ca(1)-O(5)#3	68.22(5)	O(1B)-Ca(1)-O(1W)#4	30.0(4)
O(2)#9-Ca(1)-O(5)#8	68.22(5)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z; #2 -x,-y+1,-z+1; #3 -x+1,-y+1,-z+1; #4 x,-y+1/2,z; #5 x-1,y,z-1; #6 -x,y-1/2,-z; #7 -x,y-1/2,-z+1; #8 -x+1,y-1/2,-z+1; #9 x+1,y,z+1.

Table S7. Fractional atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $CaNi_2(SeO_3)_3$. U_{eq} is defined as one third of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U_{eq}
Se1	5000	2369.5(4)	5299.7(3)	9.28(13)
Ni1	1908.6(6)	2541.8(4)	7500	7.31(13)
Se2	5000	4861.7(7)	8173.2(7)	8.53(16)
Ca1	5000	-193.1(10)	2500	12.2(2)
O1	5000	1647(2)	3802(3)	9.5(5)
O2	3281(3)	1633.7(19)	6073.5(19)	12.4(4)
O3	3180(4)	4185(3)	7500	15.6(6)
O4	5000	6208(4)	7500	20.3(9)

Table S8. Anisotropic displacement parameters (Å^2×10^3) for $CaNi_2(SeO_3)_3$. The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Se1	10.13(19)	11.1(2)	6.60(19)	-0.14(11)	0	0
Ni1	6.9(2)	6.6(2)	8.5(2)	0	0	-0.14(14)
Se2	9.5(3)	5.5(3)	10.6(3)	0.4(2)	0	0
Ca1	13.6(4)	6.7(5)	16.3(5)	0	0	0
O1	11.7(11)	9.3(12)	7.5(11)	-1.5(9)	0	0
O2	11.7(8)	13.5(9)	12.2(8)	0.0(7)	3.7(7)	-0.5(7)
O3	12.9(12)	8.8(13)	25.2(15)	0	0	-4.3(10)

O4	10.0(17)	5.4(19)	46(3)	0	0	0

Table S9. Selected bond lengths (Å) and bond angles (°) of $CaNi_2(SeO_3)_3$.

Bond	Dist.	Bond	Dist.
Se(1)-O(1)	1.723(3)	Se(2)-O(3)	1.681(3)
Se(1)-O(2)#2	1.6984(19)	Se(2)-O(4)	1.630(4)
Se(1)-O(2)	1.6983(19)	Ca(1)-O(1)	2.418(3)
Ni(1)-O(1)#3	2.132(2)	Ca(1)-O(1)#8	2.418(3)
Ni(1)-O(1)#4	2.132(2)	Ca(1)-O(2)#9	2.496(2)
Ni(1)-O(2)#5	2.035(2)	Ca(1)-O(2)#1	2.496(2)
Ni(1)-O(2)	2.035(2)	Ca(1)-O(2)#10	2.496(2)
Ni(1)-O(3)	2.032(3)	Ca(1)-O(2)#11	2.496(2)
Ni(1)-O(4)#6	2.030(3)	Ca(1)-O(3)#12	2.593(3)
Se(2)-O(3)#7	1.681(3)	Ca(1)-O(3)#3	2.593(3)
Angle	(°)	Angle	(°)
O(2)-Se(1)-O(1)	101.23(10)	O(1)#8-Ca(1)-O(2)#11	101.96(7)
O(2)#2-Se(1)-O(1)	101.23(10)	O(1)#8-Ca(1)-O(2)#1	148.22(5)
O(2)-Se(1)-O(2)#2	96.58(14)	O(1)-Ca(1)-O(2)#11	148.22(5)
O(1)#3-Ni(1)-O(1)#4	77.25(12)	O(1)-Ca(1)-O(2)#1	101.96(7)
O(2)-Ni(1)-O(1)#3	94.92(9)	O(1)#8-Ca(1)-O(2)#9	148.22(5)
O(2)#5-Ni(1)-O(1)#4	94.92(9)	O(1)-Ca(1)-O(3)#3	69.15(6)
O(2)#5-Ni(1)-O(1)#3	168.50(8)	O(1)-Ca(1)-O(3)#12	69.15(6)
O(2)-Ni(1)-O(1)#4	168.50(8)	O(1)#8-Ca(1)-O(3)#12	69.15(6)
O(2)#5-Ni(1)-O(2)	91.49(12)	O(1)#8-Ca(1)-O(3)#3	69.15(6)
O(3)-Ni(1)-O(1)#4	86.24(9)	O(2)#11-Ca(1)-O(2)#10	61.05(9)
O(3)-Ni(1)-O(1)#3	86.24(9)	O(2)#11-Ca(1)-O(2)#9	71.46(9)
O(3)-Ni(1)-O(2)#5	101.81(8)	O(2)#9-Ca(1)-O(2)#10	101.42(10)

O(3)-Ni(1)-O(2)	101.81(8)	O(2)#11-Ca(1)-O(2)#1	101.42(10)
O(4)#6-Ni(1)-O(1)#4	80.97(9)	O(2)#9-Ca(1)-O(2)#1	61.05(9)
O(4)#6-Ni(1)-O(1)#3	80.97(9)	O(2)#10-Ca(1)-O(2)#1	71.46(9)
O(4)#6-Ni(1)-O(2)#5	89.55(8)	O(2)#11-Ca(1)-O(3)#12	136.84(6)
O(4)#6-Ni(1)-O(2)	89.55(8)	O(2)#1-Ca(1)-O(3)#3	136.84(6)
O(4)#6-Ni(1)-O(3)	163.59(12)	O(2)#10-Ca(1)-O(3)#12	79.08(7)
O(3)-Se(2)-O(3)#7	105.96(17)	O(2)#11-Ca(1)-O(3)#3	79.08(7)
O(4)-Se(2)-O(3)#7	103.15(10)	O(2)#9-Ca(1)-O(3)#12	136.84(6)
O(4)-Se(2)-O(3)	103.15(10)	O(2)#9-Ca(1)-O(3)#3	79.08(7)
O(1)#8-Ca(1)-O(1)	66.79(13)	O(2)#1-Ca(1)-O(3)#12	79.08(7)
O(1)-Ca(1)-O(2)#9	101.96(7)	O(2)#10-Ca(1)-O(3)#3	136.84(6)
O(1)#8-Ca(1)-O(2)#10	101.96(7)	O(3)#12-Ca(1)-O(3)#3	129.52(13)
O(1)-Ca(1)-O(2)#10	148.22(5)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1; #2 -x+1,y,z; #3 -x+1/2,-y+1/2,-z+1; #4 -x+1/2,-y+1/2,z+1/2; #5 x,y,-z+3/2; #6 x-1/2,y-1/2,z; #7 -x+1,y,-z+3/2; #8 x,y,-z+1/2; #9 x,-y,-z+1; #10 -x+1,-y,z-1/2; #11 x,-y,z-1/2; #12 x+1/2,-y+1/2,z-1/2; #13 x+1/2,y+1/2,z; #14 -x+1/2,y+1/2,-z+3/2.