Supporting Information

Synthesis, structure and magnetic properties of two new spin-chain compounds $Ca_2Ni(HSeO_3)_2(SeO_3)_2$ and $Na_2Cu(SeO_3)_2·2H_2O$

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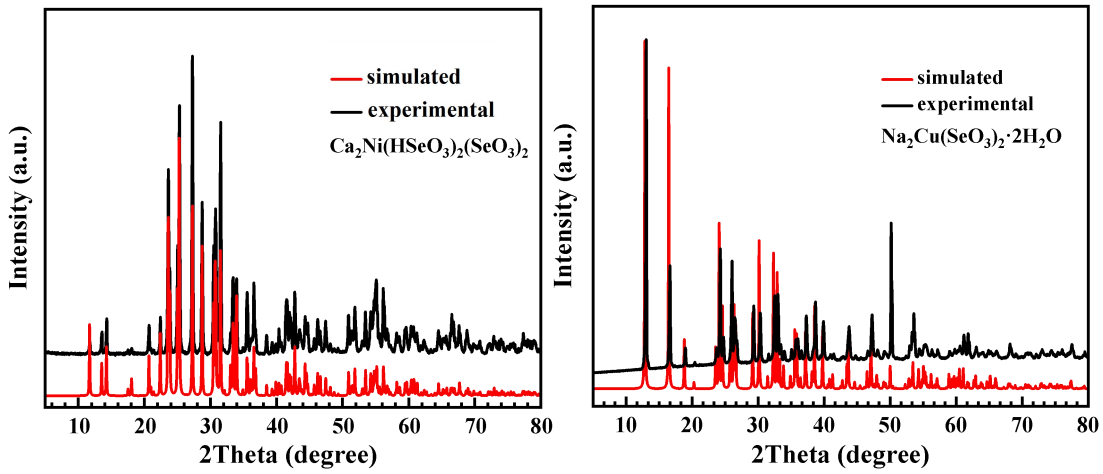
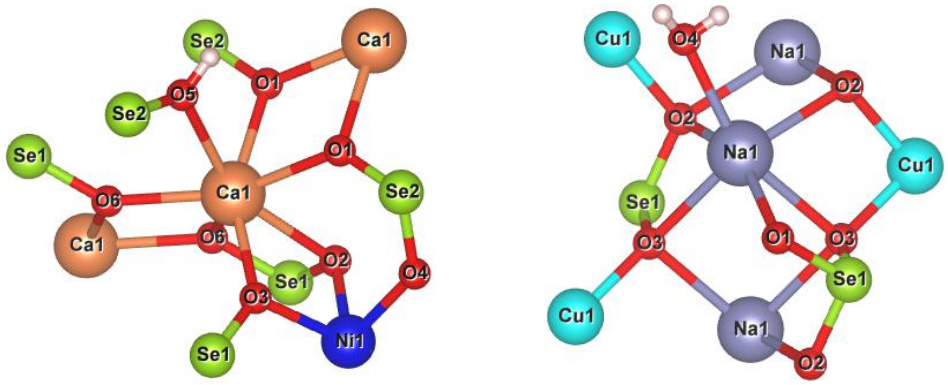


(a) (b)

Fig. S1. The powder XRD patterns of (a) $Ca_2Ni(HSeO_3)_2(SeO_3)_2$ and (b) $Na_2Cu(SeO_3)_2{\cdot}2H_2O$.



(a) (b)

Fig. S2. The oxygen-coordination environments for (a) Ca atom in $Ca_2Ni(HSeO_3)_2(SeO_3)_2$ and (b) Na atom in $Na_2Cu(SeO_3)_2{\cdot}2H_2O$.

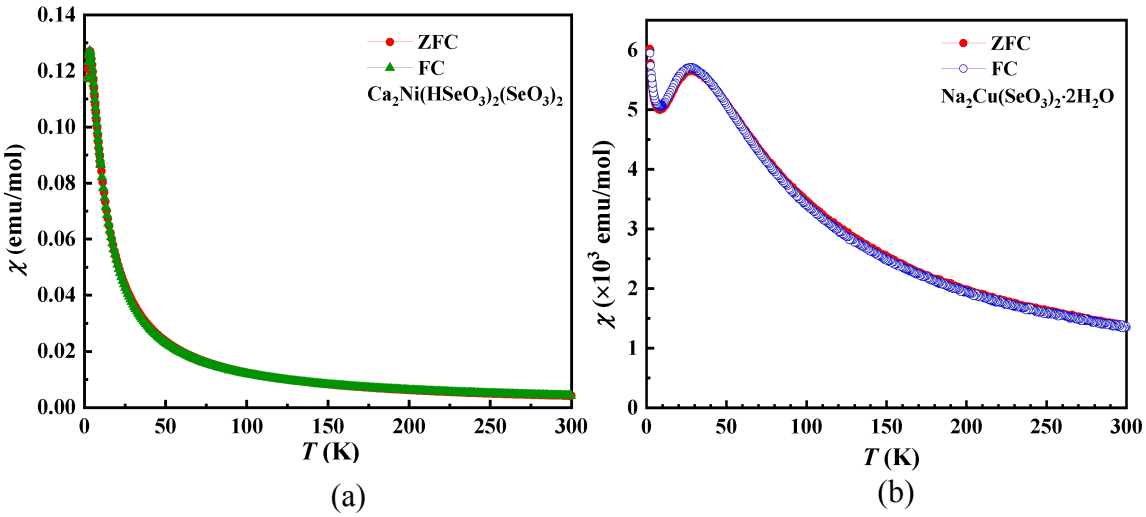


Fig. S3. The FC-ZFC magnetic susceptibilities for (a) $Ca_2Ni(HSeO_3)_2(SeO_3)_2$ and (b) $Na_2Cu(SeO_3)_2{\cdot}2H_2O$.

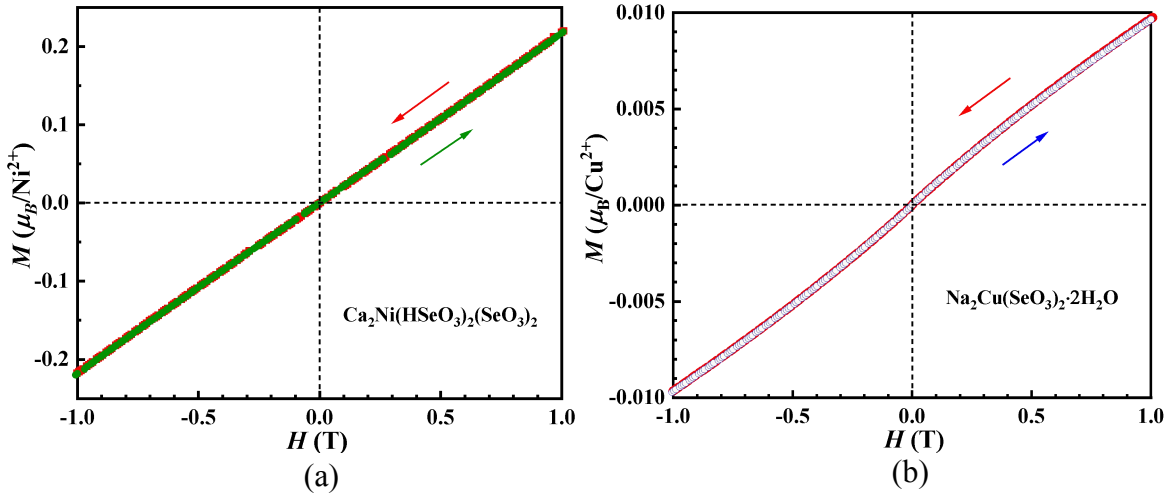


Fig. S4. The magnetization curves at low magnetic field for (a) $Ca_2Ni(HSeO_3)_2(SeO_3)_2$ and (b) $Na_2Cu(SeO_3)_2{\cdot}2H_2O$.

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$ Å^2) for $Ca_2Ni(HSeO_3)_2(SeO_3)_2$. U_{eq} is defined as one third of the trace of the orthogonalised U_{ij} tensor.

atom	x	y	z	U_{eq}
Se(1)	-706(1)	2386(1)	3192(1)	8(1)
Se(2)	7086(1)	1897(1)	7246(1)	10(1)
Ni(1)	5000	5000	5000	8(1)
Ca(1)	3829(1)	2718(1)	472(1)	9(1)
O(1)	6350(4)	3716(3)	8885(3)	14(1)
O(2)	-2517(4)	4395(3)	3333(3)	10(1)
O(3)	1953(4)	3298(3)	2763(3)	11(1)
O(4)	5771(4)	2353(3)	5427(3)	14(1)
O(5)	10545(4)	2704(4)	7739(3)	16(1)
O(6)	-2516(4)	782(3)	1167(3)	15(1)
H(5)	10960(120)	3660(90)	7400(90)	65(19)

Table S2. Selected bond lengths (Å) and bond angles (°) of $Ca_2Ni(HSeO_3)_2(SeO_3)_2$.

Bond	Dist.	Bond	Dist.
Se(1)–O(2)	1.719(2)	Ni(1)–O(3)#5	2.0758(19)
Se(1)–O(3)	1.6989(19)	Ni(1)–O(4)	2.051(2)
Se(1)–O(6)	1.685(2)	Ni(1)–O(4)#5	2.051(2)
Se(2)–O(1)	1.665(2)	Ca(1)–O(1)#6	2.361(2)
Se(2)–O(4)	1.653(2)	Ca(1)–O(1)#5	2.387(2)
Se(2)–O(5)	1.793(2)	Ca(1)–O(2)#4	2.527(2)
Ni(1)–O(2)#3	2.109(2)	Ca(1)–O(5)#9	2.493(2)
Ni(1)–O(2)#4	2.109(2)	Ca(1)–O(6)#4	2.463(2)
Ni(1)–O(3)	2.0758(19)	Ca(1)–O(6)#10	2.341(2)
		Ca(1)-O(3)	2.311(2)
Angle	(°)	Angle	(°)
O(3)-Se(1)-O(2)	99.97(10)	O(1)#8-Ca(1)-O(1)#5	73.19(8)
O(6)-Se(1)-O(2)	97.58(10)	O(1)#8-Ca(1)-O(2)#4	91.05(7)
O(6)-Se(1)-O(3)	102.40(10)	O(1)#5-Ca(1)-O(2)#4	76.64(7)
O(1)-Se(2)-O(5)	100.58(11)	O(1)#8-Ca(1)-O(5)#9	74.80(8)
O(4)-Se(2)-O(1)	106.37(11)	O(1)#5-Ca(1)-O(5)#9	78.05(8)
O(4)-Se(2)-O(5)	103.12(11)	O(1)#8-Ca(1)-O(6)#4	84.69(8)
O(2)#3-Ni(1)-O(2)#4	180	O(1)#5-Ca(1)-O(6)#4	132.26(8)
O(3)-Ni(1)-O(2)#4	86.65(8)	O(3)-Ca(1)-O(1)#5	83.10(8)
O(3)#5-Ni(1)-O(2)#3	86.65(8)	O(3)-Ca(1)-O(1)#8	153.91(8)
O(3)#5-Ni(1)-O(2)#4	93.35(8)	O(3)-Ca(1)-O(2)#4	72.65(7)
O(3)-Ni(1)-O(2)#3	93.35(8)	O(3)-Ca(1)-O(5)#9	111.24(7)
O(3)-Ni(1)-O(3)#5	180.00(9)	O(3)-Ca(1)-O(6)#4	104.15(8)
O(4)-Ni(1)-O(2)#4	89.04(8)	O(3)-Ca(1)-O(6)#10	102.80(8)
O(4)#5-Ni(1)-O(2)#3	89.04(8)	O(5)#9-Ca(1)-O(2)#4	153.69(8)
O(4)#5-Ni(1)-O(2)#4	90.96(8)	O(6)#10-Ca(1)-O(1)#5	155.45(8)
O(4)-Ni(1)-O(2)#3	90.96(8)	O(6)#10-Ca(1)-O(1)#8	103.29(8)
O(4)-Ni(1)-O(3)#5	91.30(8)	O(6)#10-Ca(1)-O(2)#4	127.91(7)
O(4)-Ni(1)-O(3)	88.70(8)	O(6)#4-Ca(1)-O(2)#4	61.74(7)
O(4)#5-Ni(1)-O(3)#5	88.70(8)	O(6)#4-Ca(1)-O(5)#9	136.24(8)
O(4)#5-Ni(1)-O(3)	91.30(8)	O(6)#10-Ca(1)-O(5)#9	77.62(8)
O(4)#5-Ni(1)-O(4)	180	O(6)#10-Ca(1)-O(6)#4	70.00(8)

Symmetry transformations used to generate equivalent atoms:

#3 -x, -y+1, -z+1 #4 x+1, y, z #5 -x+1, -y+1, -z+1 #6 -x+1,-y+1,-z

#8 x, y, z-1 #9 x-1, y, z-1 #10 -x, -y, -z

Table S3. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\times 10^3$ Å^2) for $Na_2Cu(SeO_3)_2 \cdot 2H_2O$. U_{eq} is defined as one third of the trace of the orthogonalised U_{ij} tensor.

atom	x	y	z	U_{eq}
Se(1)	-537(1)	685(1)	2658(1)	13(1)
Cu(1)	5000	0	5000	13(1)
Na(1)	6799(2)	4873(2)	3329(1)	20(1)
O(1)	-1143(3)	2584(3)	1400(2)	21(1)
O(25)	-1508(2)	1848(2)	4607(2)	15(1)
O(3)	3061(2)	1966(2)	3747(2)	15(1)
O(4)	3489(3)	6533(3)	1913(2)	24(1)
H(4A)	2830(70)	7060(60)	1020(50)	40(8)
H(4B)	2080(80)	5310(70)	1810(50)	50(10)

Table S4. Selected bond lengths (Å) and bond angles (°) of $Na_2Cu(SeO_3)_2 \cdot 2H_2O$.

Bond	Dist.	Bond	Dist.
Se(1)-O(1)	1.6745(12)	Na(1)-O(1)#5	2.3854(16)
Se(1)-O(25)	1.7193(12)	Na(1)-O(25)#5	2.4748(13)
Se(1)-O(3)	1.7071(11)	Na(1)-O(25)#2	2.5046(15)
Cu(1)-O(25)#5	1.9873(11)	Na(1)-O(3)	2.3717(14)
Cu(1)-O(25)#6	1.9873(11)	Na(1)-O(3)#2	2.4930(15)
Cu(1)-O(3)#3	1.9799(11)	Na(1)-O(4)	2.3495(15)
Cu(1)-O(3)	1.9800(11)		
Angle	(°)	Angle	(°)
O(1)-Se(1)-O(25)	100.00(6)	O(25)#5-Na(1)-O(25)#2	88.43(5)
O(1)-Se(1)-O(3)	100.95(6)	O(25)#5-Na(1)-O(3)#2	104.48(5)
O(3)-Se(1)-O(25)	98.77(6)	O(3)-Na(1)-O(1)#5	107.65(5)
O(25)#6-Cu(1)-O(25)#5	180	O(3)-Na(1)-O(25)#2	138.00(5)
O(3)-Cu(1)-O(25)#6	92.11(5)	O(3)#2-Na(1)-O(25)#2	62.72(4)
O(3)-Cu(1)-O(25)#5	87.89(5)	O(3)-Na(1)-O(25)#5	69.19(4)
O(3)#3-Cu(1)-O(25)#5	92.11(5)	O(3)-Na(1)-O(3)#2	88.23(5)
O(3)#3-Cu(1)-O(25)#6	87.89(5)	O(4)-Na(1)-O(1)#5	120.60(6)
O(3)#3-Cu(1)-O(3)	180	O(4)-Na(1)-O(25)#2	112.48(6)
O(1)#5-Na(1)-O(25)#2	92.68(5)	O(4)-Na(1)-O(25)#5	157.21(6)
O(1)#5-Na(1)-O(25)#5	64.65(4)	O(4)-Na(1)-O(3)	88.59(5)
O(1)#5-Na(1)-O(3)#2	154.16(5)	O(4)-Na(1)-O(3)#2	78.96(5)

Symmetry transformations used to generate equivalent atoms:

#2 -x+1,-y+1,-z+1 #3 -x+1,-y,-z+1 #5 x+1,y,z #6 -x,-y,-z+1