

Supporting Information

**Synthesis and magnetic properties of new tellurate compounds**

**Na<sub>4</sub>MTeO<sub>6</sub> (M = Co and Ni) with a ferromagnetic spin chain structure**

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**Figure S1.** The thermal behaviors of of Na<sub>4</sub>MTeO<sub>6</sub> (M = Co, Ni).

**Figure S2.** Simulated and experimental powder X-ray (Cu K $\alpha$ ) diffraction patterns of Na<sub>4</sub>MTeO<sub>6</sub> (M = Co, Ni).

**Figure S3.** The oxygen-coordination environments for (a) Co and (b) Te atoms of Na<sub>4</sub>CoTeO<sub>6</sub>, respectively.

**Figure S4.** The oxygen-coordination environments for (a) Ni and (b) Te atoms of Na<sub>4</sub>NiTeO<sub>6</sub>, respectively.

**Table S1.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for Na<sub>4</sub>CoTeO<sub>6</sub> and Na<sub>4</sub>NiTeO<sub>6</sub>.

**Table S2.** Bond lengths [ $\text{\AA}$ ] and angles [deg] for Na<sub>4</sub>CoTeO<sub>6</sub>.

**Table S3.** Bond lengths [ $\text{\AA}$ ] and angles [deg] for Na<sub>4</sub>NiTeO<sub>6</sub>.

**Table S4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for for Na<sub>4</sub>CoTeO<sub>6</sub> and Na<sub>4</sub>NiTeO<sub>6</sub>.

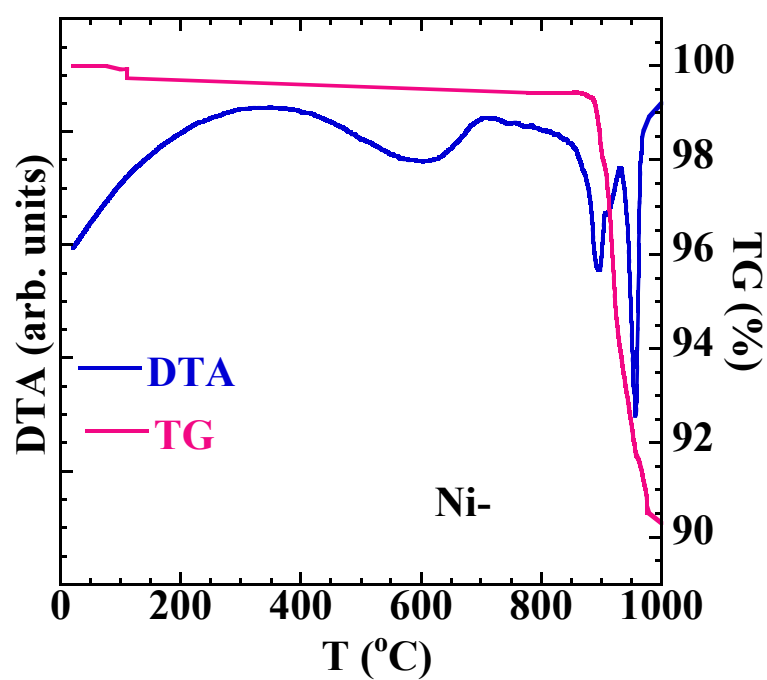
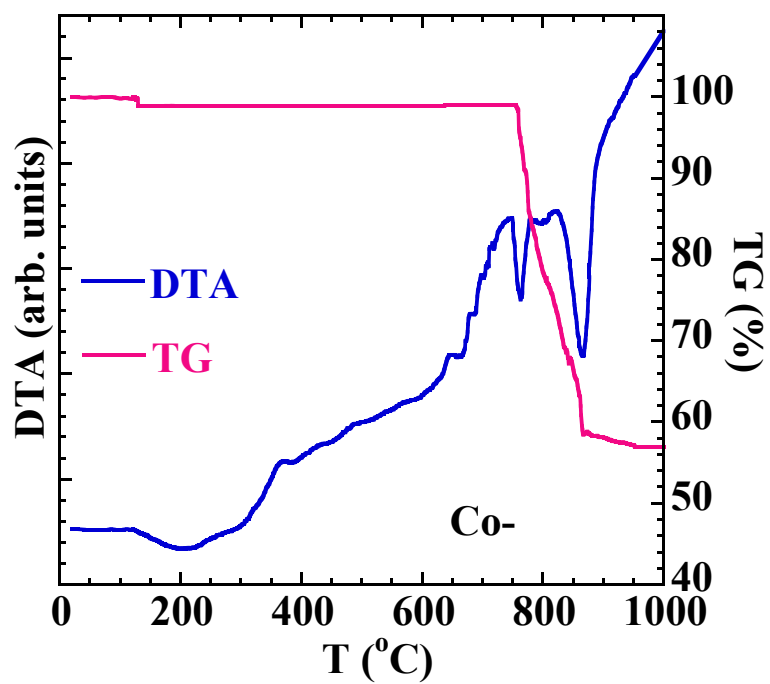
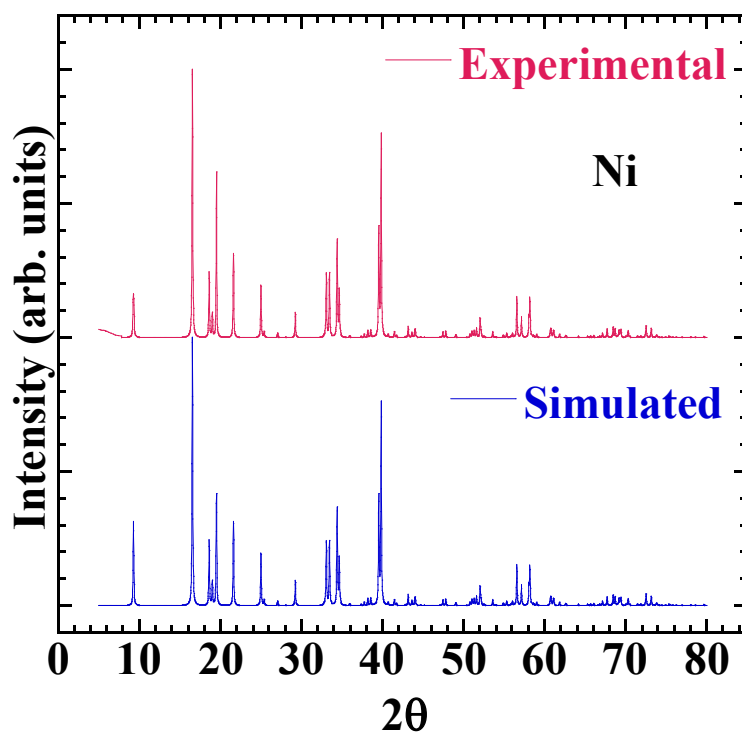
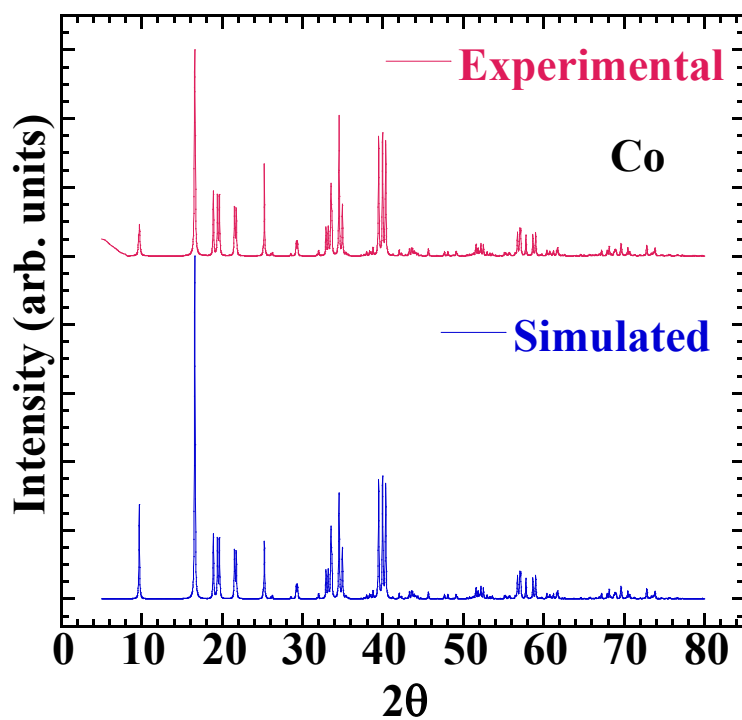
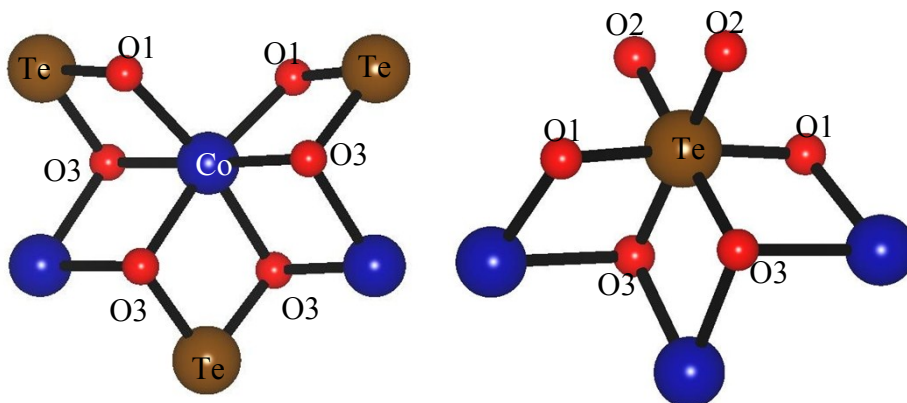


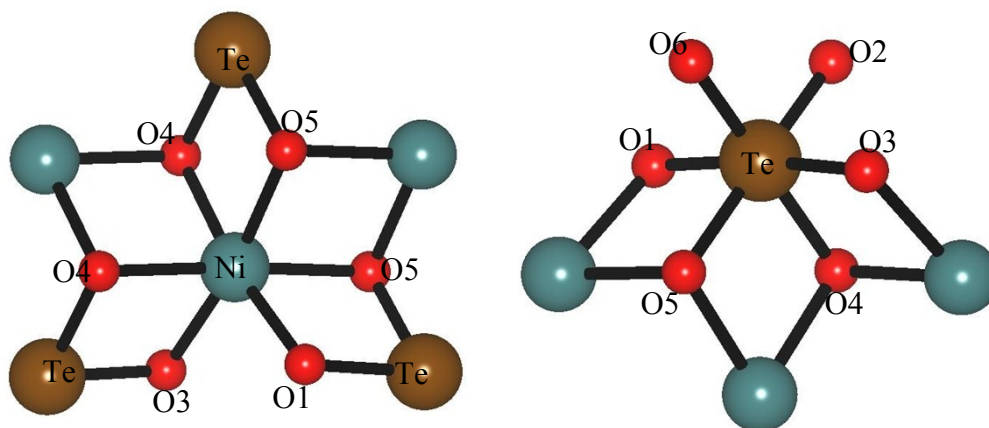
Figure S1. The thermal behaviors of  $\text{Na}_4\text{MTeO}_6$  ( $\text{M} = \text{Co}, \text{Ni}$ ).



**Figure S2.** Simulated (blue line) and experimental (red line) powder X-ray (Cu K $\alpha$ ) diffraction patterns of Na<sub>4</sub>MTeO<sub>6</sub> (M = Co, Ni).



**Figure S3.** The oxygen-coordination environments for (a) Co and (b) Te atoms of  $\text{Na}_4\text{CoTeO}_6$ , respectively.



**Figure S4.** The oxygen-coordination environments for (a) Ni and (b) Te atoms of  $\text{Na}_4\text{NiTeO}_6$ , respectively.

**Table S1.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{Na}_4\text{CoTeO}_6$  and  $\text{Na}_4\text{NiTeO}_6$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

atom	x	y	z	$U(\text{eq})$
Te(1)	5000	2566(1)	7500	6(1)
Co(1)	5000	5853(1)	7500	8(1)
O(1)	2988(5)	4093(2)	5308(5)	8(1)
O(2)	6986(5)	2679(2)	5231(5)	8(1)
O(3)	2816(5)	1184(3)	5415(5)	8(1)
Na(1)	5000	815(2)	2500	5(1)
Na(2)	0	5721(2)	2500	12(1)
Na(3)	0	2577(2)	2500	18(1)
Na(4)	0	820(2)	7500	19(1)
Te(1)	2481(1)	9927(1)	2431(1)	3(1)
Ni(1)	2503(1)	10029(1)	-826(1)	5(1)
O(1)	-861(3)	11981(3)	1987(2)	6(1)
O(2)	3473(3)	12087(3)	3426(2)	7(1)
O(3)	5813(3)	7872(3)	2668(2)	6(1)
O(4)	3727(3)	11937(3)	563(2)	6(1)
O(5)	1259(3)	8029(3)	1214(2)	6(1)
O(6)	1461(3)	7745(3)	4183(2)	7(1)
Na(1)	0	5000	0	11(1)
Na(2)	5070(2)	4930(2)	1570(1)	10(1)
Na(3)	9806(2)	4934(2)	3307(1)	11(1)
Na(4)	5000	5000	5000	24(1)
Na(5)	2518(1)	39(1)	5803(1)	6(1)

**Table S2.** Bond lengths [ $\text{\AA}$ ] and angles [deg] for  $\text{Na}_4\text{CoTeO}_6$ .

Te(1)-O(3)	1.906(3)	Te(1)-O(2)#1	1.941(3)
Te(1)-O(3)#1	1.906(3)	Te(1)-O(1)#1	1.988(3)
Te(1)-O(2)	1.941(3)	Te(1)-O(1)	1.988(3)
Co(1)-O(2)#6	2.084(3)	Co(1)-O(1)#1	2.155(3)
Co(1)-O(2)#5	2.084(3)	Co(1)-O(1)#6	2.203(3)
Co(1)-O(1)	2.155(3)	Co(1)-O(1)#5	2.203(3)
Na(1)-O(2)#10	2.354(3)	Na(1)-O(3)#3	2.351(3)
Na(1)-O(3)#11	2.351(3)	Na(1)-O(3)#10	2.354(3)
O(2)-Na(1)	2.354(3)	O(3)-Na(1)	2.354(3)
Na(2)-O(2)#5	2.319(3)	Na(2)-O(1)#7	2.390(3)
Na(2)-O(2)#14	2.319(3)	Na(2)-O(1)#16	2.431(3)
Na(2)-O(1)#15	2.390(3)	O(1)-Na(2)	2.431(3)
Na(3)-O(3)#16	2.273(3)	Na(3)-O(2)#10	2.625(3)
Na(3)-O(1)#16	2.365(3)	Na(3)-O(2)#18	2.625(3)
O(3)-Na(3)	2.273(3)	O(1)-Na(3)	2.365(3)
Na(4)-O(3)#19	2.281(3)	Na(4)-O(3)#9	2.655(3)
Na(4)-O(2)#1	2.489(3)	Na(4)-O(3)#20	2.655(3)
Na(4)-O(2)#18	2.489(3)	O(3)-Na(4)	2.281(3)
O(3)-Te(1)-O(3)#1	92.65(16)	O(2)-Te(1)-O(1)#1	90.44(12)
O(3)-Te(1)-O(2)	93.12(12)	O(2)#1-Te(1)-O(1)#1	84.89(12)
O(3)#1-Te(1)-O(2)	91.28(12)	O(3)-Te(1)-O(1)	90.83(12)
O(3)-Te(1)-O(2)#1	91.28(12)	O(3)#1-Te(1)-O(1)	174.96(9)
O(3)#1-Te(1)-O(2)#1	93.12(12)	O(2)-Te(1)-O(1)	84.89(12)
O(2)-Te(1)-O(2)#1	173.62(14)	O(2)#1-Te(1)-O(1)	90.44(12)
O(3)-Te(1)-O(1)#1	174.96(9)	O(1)#1-Te(1)-O(1)	85.93(15)
O(3)#1-Te(1)-O(1)#1	90.83(12)	O(2)#5-Co(1)-O(1)#6	101.81(11)
O(2)#6-Co(1)-O(2)#5	95.76(14)	O(1)-Co(1)-O(1)#6	96.09(10)
O(2)#6-Co(1)-O(1)	169.07(10)	O(1)#1-Co(1)-O(1)#6	85.98(11)
O(2)#5-Co(1)-O(1)	93.52(11)	O(2)#6-Co(1)-O(1)#5	101.81(11)
O(2)#6-Co(1)-O(1)#1	93.52(11)	O(2)#5-Co(1)-O(1)#5	76.37(12)
O(2)#5-Co(1)-O(1)#1	169.07(10)	O(1)-Co(1)-O(1)#5	85.98(11)
O(1)-Co(1)-O(1)#1	77.89(14)	O(1)#1-Co(1)-O(1)#5	96.09(10)
O(2)#6-Co(1)-O(1)#6	76.37(12)	O(1)#6-Co(1)-O(1)#5	177.34(12)
O(2)-Na(1)-O(2)#10	82.08(14)	O(3)#11-Na(1)-O(3)	98.01(11)
O(2)-Na(1)-O(3)#11	169.61(9)	O(3)#3-Na(1)-O(3)	95.88(10)
O(2)#10-Na(1)-O(3)#11	103.78(10)	O(2)-Na(1)-O(3)#10	94.05(11)
O(2)-Na(1)-O(3)#3	103.78(10)	O(2)#10-Na(1)-O(3)#10	72.79(11)
O(2)#10-Na(1)-O(3)#3	169.61(9)	O(3)#11-Na(1)-O(3)#10	95.88(10)
O(3)#11-Na(1)-O(3)#3	71.81(14)	O(3)#3-Na(1)-O(3)#10	98.01(11)
O(2)-Na(1)-O(3)	72.79(11)	O(3)-Na(1)-O(3)#10	162.83(15)
O(2)#10-Na(1)-O(3)	94.05(11)	O(2)#14-Na(2)-O(1)#16	81.07(10)
O(2)#5-Na(2)-O(2)#14	97.85(15)	O(1)#15-Na(2)-O(1)#16	101.00(10)

O(2)#5-Na(2)-O(1)#15	72.60(11)	O(1)#7-Na(2)-O(1)#16	84.48(11)
O(2)#14-Na(2)-O(1)#15	101.63(11)	O(2)#5-Na(2)-O(1)	81.07(10)
O(2)#5-Na(2)-O(1)#7	101.63(11)	O(2)#14-Na(2)-O(1)	173.23(9)
O(2)#14-Na(2)-O(1)#7	72.60(11)	O(1)#15-Na(2)-O(1)	84.48(11)
O(1)#15-Na(2)-O(1)#7	171.49(14)	O(1)#7-Na(2)-O(1)	101.00(10)
O(2)#5-Na(2)-O(1)#16	173.23(9)	O(1)#16-Na(2)-O(1)	100.77(14)
O(3)#16-Na(3)-O(3)	108.59(16)	O(1)-Na(3)-O(2)#10	83.48(10)
O(3)#16-Na(3)-O(1)	176.32(8)	O(1)#16-Na(3)-O(2)#10	93.91(11)
O(3)-Na(3)-O(1)	73.43(11)	O(3)#16-Na(3)-O(2)#18	89.07(10)
O(3)#16-Na(3)-O(1)#16	73.43(11)	O(3)-Na(3)-O(2)#18	93.42(10)
O(3)-Na(3)-O(1)#16	176.32(8)	O(1)-Na(3)-O(2)#18	93.91(11)
O(1)-Na(3)-O(1)#16	104.73(15)	O(1)#16-Na(3)-O(2)#18	83.48(10)
O(3)#16-Na(3)-O(2)#10	93.42(10)	O(2)#10-Na(3)-O(2)#18	175.75(13)
O(3)-Na(3)-O(2)#10	89.07(10)	O(3)#19-Na(4)-O(3)#9	91.68(11)
O(3)-Na(4)-O(3)#19	162.51(17)	O(2)#1-Na(4)-O(3)#9	171.19(8)
O(3)-Na(4)-O(2)#1	70.28(11)	O(2)#18-Na(4)-O(3)#9	91.99(10)
O(3)#19-Na(4)-O(2)#1	96.95(11)	O(3)-Na(4)-O(3)#20	91.68(11)
O(3)-Na(4)-O(2)#18	96.95(11)	O(3)#19-Na(4)-O(3)#20	100.90(10)
O(3)#19-Na(4)-O(2)#18	70.28(11)	O(2)#1-Na(4)-O(3)#20	91.99(10)
O(2)#1-Na(4)-O(2)#18	89.27(14)	O(2)#18-Na(4)-O(3)#20	171.19(8)
O(3)-Na(4)-O(3)#9	100.90(10)	O(3)#9-Na(4)-O(3)#20	88.09(13)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, y, -z+3/2$	#2 $x, y, z+1$	#3 $-x+1, -y, -z+1$
#4 $x+1, y, z+1$	#5 $-x+1, -y+1, -z+1$	#6 $x, -y+1, z+1/2$
#7 $-x, -y+1, -z+1$	#8 $x+1, y, z$	#9 $-x, -y, -z+1$
#10 $-x+1, y, -z+1/2$	#11 $x, -y, z-1/2$	#12 $-x+1, -y, -z$
#13 $x, y, z-1$	#14 $x-1, -y+1, z-1/2$	#15 $x, -y+1, z-1/2$
#16 $-x, y, -z+1/2$	#17 $-x, -y+1, -z$	#18 $x-1, y, z$
#19 $-x, y, -z+3/2$	#20 $x, -y, z+1/2$	#21 $-x, -y, -z+2$

**Table S3.** Bond lengths [Å] and angles [deg] for Na<sub>4</sub>NiTeO<sub>6</sub>.

Te(1)-O(2)	1.8962(15)	Te(1)-O(1)	1.9550(16)
Te(1)-O(6)	1.9089(16)	Te(1)-O(5)	1.9813(16)
Te(1)-O(3)	1.9506(16)	Te(1)-O(4)	1.9991(16)
Ni(1)-O(1)#1	2.0989(16)	Ni(1)-O(5)	2.1194(17)
Ni(1)-O(3)#2	2.1121(16)	Ni(1)-O(5)#1	2.1237(17)
Ni(1)-O(4)	2.1124(16)	Ni(1)-O(4)#2	2.1321(17)
Na(1)-O(1)#1	2.2609(16)	Na(1)-O(4)#1	2.3807(16)
Na(1)-O(1)#10	2.2609(16)	Na(1)-O(5)#11	2.5142(16)
Na(1)-O(4)#10	2.3807(16)	O(5)-Na(1)	2.5142(16)
Na(2)-O(2)#10	2.2944(18)	Na(2)-O(4)#2	2.4476(19)
Na(2)-O(4)#10	2.3878(18)	Na(2)-O(1)#12	2.4877(18)
O(5)-Na(2)	2.4296(19)	O(3)-Na(2)	2.3012(18)
Na(3)-O(6)#13	2.3029(18)	Na(3)-O(5)#13	2.4679(19)
Na(3)-O(2)#12	2.3194(18)	Na(3)-O(6)#4	2.595(2)
Na(3)-O(1)#12	2.4422(18)	O(3)-Na(3)	2.4564(19)
Na(4)-O(6)#4	2.2384(16)	Na(4)-O(2)#10	2.7559(16)
Na(4)-O(3)#4	2.4343(17)	Na(4)-O(2)#15	2.7559(16)
O(3)-Na(4)	2.4343(17)	O(6)-Na(4)	2.2384(16)
Na(5)-O(6)#3	2.3057(18)	Na(5)-O(1)#3	2.3424(19)
Na(5)-O(2)#4	2.3074(18)	Na(5)-O(3)#4	2.3956(18)
Na(5)-O(2)#10	2.3296(19)	Na(5)-O(6)#10	2.4191(18)
O(2)-Te(1)-O(6)	92.87(7)	O(3)-Te(1)-O(5)	91.24(7)
O(2)-Te(1)-O(3)	93.30(7)	O(1)-Te(1)-O(5)	84.32(7)
O(6)-Te(1)-O(3)	91.09(7)	O(2)-Te(1)-O(4)	90.42(7)
O(2)-Te(1)-O(1)	90.80(7)	O(6)-Te(1)-O(4)	174.84(6)
O(6)-Te(1)-O(1)	92.86(7)	O(3)-Te(1)-O(4)	84.75(7)
O(3)-Te(1)-O(1)	174.16(6)	O(1)-Te(1)-O(4)	91.06(7)
O(2)-Te(1)-O(5)	173.28(6)	O(5)-Te(1)-O(4)	85.07(7)
O(6)-Te(1)-O(5)	91.99(7)	O(3)#2-Ni(1)-O(5)#1	100.26(6)
O(1)#1-Ni(1)-O(3)#2	94.55(7)	O(4)-Ni(1)-O(5)#1	97.69(6)
O(1)#1-Ni(1)-O(4)	171.45(6)	O(5)-Ni(1)-O(5)#1	85.12(6)
O(3)#2-Ni(1)-O(4)	93.24(7)	O(1)#1-Ni(1)-O(4)#2	99.99(6)
O(1)#1-Ni(1)-O(5)	93.50(7)	O(3)#2-Ni(1)-O(4)#2	77.70(6)
O(3)#2-Ni(1)-O(5)	171.14(6)	O(4)-Ni(1)-O(4)#2	85.09(6)
O(4)-Ni(1)-O(5)	78.97(7)	O(5)-Ni(1)-O(4)#2	97.24(6)
O(1)#1-Ni(1)-O(5)#1	77.47(6)	O(5)#1-Ni(1)-O(4)#2	176.67(5)
O(1)#1-Na(1)-O(1)#10	180.00(6)	O(4)#10-Na(1)-O(5)	98.72(5)
O(1)#1-Na(1)-O(4)#10	105.16(6)	O(4)#1-Na(1)-O(5)	81.28(5)
O(1)#10-Na(1)-O(4)#10	74.84(6)	O(1)#1-Na(1)-O(5)#11	100.10(6)
O(1)#1-Na(1)-O(4)#1	74.84(6)	O(1)#10-Na(1)-O(5)#11	79.90(6)
O(1)#10-Na(1)-O(4)#1	105.16(6)	O(4)#10-Na(1)-O(5)#11	81.28(5)
O(4)#10-Na(1)-O(4)#1	180.00(5)	O(4)#1-Na(1)-O(5)#11	98.72(5)



O(1)#1-Na(1)-O(5)	79.90(6)	O(5)-Na(1)-O(5)#11	180.00(5)
O(1)#10-Na(1)-O(5)	100.10(6)	O(3)-Na(2)-O(4)#2	80.51(6)
O(2)#10-Na(2)-O(3)	102.56(7)	O(4)#10-Na(2)-O(4)#2	103.86(6)
O(2)#10-Na(2)-O(4)#10	72.37(6)	O(5)-Na(2)-O(4)#2	81.70(6)
O(3)-Na(2)-O(4)#10	171.99(6)	O(2)#10-Na(2)-O(1)#12	88.77(6)
O(2)#10-Na(2)-O(5)	93.17(6)	O(3)-Na(2)-O(1)#12	103.03(6)
O(3)-Na(2)-O(5)	72.83(6)	O(4)#10-Na(2)-O(1)#12	83.30(6)
O(4)#10-Na(2)-O(5)	100.93(6)	O(5)-Na(2)-O(1)#12	175.72(6)
O(2)#10-Na(2)-O(4)#2	173.03(6)	O(4)#2-Na(2)-O(1)#12	96.67(6)
O(6)#13-Na(3)-O(2)#12	98.06(7)	O(1)#12-Na(3)-O(5)#13	96.53(6)
O(6)#13-Na(3)-O(1)#12	163.63(6)	O(3)-Na(3)-O(5)#13	82.63(6)
O(2)#12-Na(3)-O(1)#12	70.28(6)	O(6)#13-Na(3)-O(6)#4	96.46(6)
O(6)#13-Na(3)-O(3)	90.05(6)	O(2)#12-Na(3)-O(6)#4	90.99(6)
O(2)#12-Na(3)-O(3)	168.07(7)	O(1)#12-Na(3)-O(6)#4	95.21(6)
O(1)#12-Na(3)-O(3)	99.92(6)	O(3)-Na(3)-O(6)#4	96.81(6)
O(6)#13-Na(3)-O(5)#13	71.73(7)	O(5)#13-Na(3)-O(6)#4	168.17(6)
O(2)#12-Na(3)-O(5)#13	91.57(6)	O(6)#4-Na(4)-O(2)#10	91.97(6)
O(6)-Na(4)-O(6)#4	180.00(8)	O(3)-Na(4)-O(2)#10	87.16(6)
O(6)-Na(4)-O(3)	72.12(6)	O(3)#4-Na(4)-O(2)#10	92.84(6)
O(6)#4-Na(4)-O(3)	107.88(6)	O(6)-Na(4)-O(2)#15	91.97(6)
O(6)-Na(4)-O(3)#4	107.88(6)	O(6)#4-Na(4)-O(2)#15	88.03(6)
O(6)#4-Na(4)-O(3)#4	72.12(6)	O(3)-Na(4)-O(2)#15	92.84(6)
O(3)-Na(4)-O(3)#4	180.0	O(3)#4-Na(4)-O(2)#15	87.16(6)
O(6)-Na(4)-O(2)#10	88.03(6)	O(2)#10-Na(4)-O(2)#15	180.00(5)
O(6)#3-Na(5)-O(2)#4	160.80(6)	O(2)#10-Na(5)-O(3)#4	105.70(7)
O(6)#3-Na(5)-O(2)#10	98.46(6)	O(1)#3-Na(5)-O(3)#4	81.52(7)
O(2)#4-Na(5)-O(2)#10	96.65(6)	O(6)#3-Na(5)-O(6)#10	96.52(6)
O(6)#3-Na(5)-O(1)#3	74.07(6)	O(2)#4-Na(5)-O(6)#10	99.56(6)
O(2)#4-Na(5)-O(1)#3	92.10(6)	O(2)#10-Na(5)-O(6)#10	70.96(6)
O(2)#10-Na(5)-O(1)#3	169.98(7)	O(1)#3-Na(5)-O(6)#10	102.82(7)
O(6)#3-Na(5)-O(3)#4	91.51(6)	O(3)#4-Na(5)-O(6)#10	171.66(6)
O(2)#4-Na(5)-O(3)#4	72.98(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z	#2 -x+1,-y+2,-z	#3 -x,-y+1,-z+1
#4 -x+1,-y+1,-z+1	#5 x,y+1,z	#6 -x+1,-y+1,-z
#7 x,y+1,z-1	#8 x-1,y+1,z	#9 x-1,y,z
#10 x,y-1,z	#11 -x,-y+1,-z	#12 x+1,y-1,z
#13 x+1,y,z	#14 -x+1,-y,-z+1	#15 -x+1,-y+2,-z+1
#16 -x,-y,-z+1		

**Table S4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for for  $\text{Na}_4\text{CoTeO}_6$  and  $\text{Na}_4\text{NiTeO}_6$ . The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U11 + \dots + 2 h k a^* b^* U12 ]$ .

atom	U11	U22	U33	U23	U13	U12
Te(1)	5(1)	8(1)	4(1)	0	1(1)	0
Co(1)	8(1)	9(1)	6(1)	0	2(1)	0
O(1)	6(1)	11(1)	6(1)	1(1)	2(1)	1(1)
O(2)	6(1)	13(1)	7(1)	0(1)	4(1)	0(1)
O(3)	7(1)	11(1)	6(1)	-4(1)	2(1)	-2(1)
Na(1)	6(1)	7(1)	3(1)	0	3(1)	0
Na(2)	10(1)	15(1)	11(1)	0	5(1)	0
Na(3)	15(1)	16(1)	16(1)	0	-4(1)	0
Na(4)	16(1)	24(2)	21(1)	0	11(1)	0
Te(1)	3(1)	2(1)	4(1)	-1(1)	0(1)	0(1)
Ni(1)	5(1)	5(1)	6(1)	-2(1)	0(1)	-1(1)
O(1)	4(1)	5(1)	8(1)	-3(1)	0(1)	1(1)
O(2)	9(1)	6(1)	8(1)	-4(1)	0(1)	-2(1)
O(3)	5(1)	5(1)	8(1)	-1(1)	-1(1)	2(1)
O(4)	7(1)	5(1)	4(1)	-1(1)	1(1)	-2(1)
O(5)	6(1)	6(1)	7(1)	-3(1)	0(1)	-1(1)
O(6)	9(1)	5(1)	6(1)	0(1)	1(1)	-1(1)
Na(1)	11(1)	8(1)	11(1)	2(1)	1(1)	1(1)
Na(2)	11(1)	7(1)	11(1)	-3(1)	0(1)	-2(1)
Na(3)	11(1)	9(1)	15(1)	-5(1)	-1(1)	-1(1)
Na(4)	13(1)	23(1)	21(1)	12(1)	4(1)	10(1)
Na(5)	5(1)	8(1)	6(1)	-1(1)	0(1)	0(1)