Supplementary Materials

The open framework compound $Ni_{15}Te_{12}O_{34}Cl_{10}$ - synthesis, crystal structure and magnetic properties

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Table S1 Atomic coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $Ni_{15}Te_{12}O_{34}Cl_{10}$.

Atom	*x*	*y*	*z*	*U*(eq)
Te(1)	0.92985(4)	0.93140(4)	-0.18534(4)	0.00705(11)
Te(2)	0.89314(4)	0.81794(4)	0.25306(4)	0.00819(11)
Te(3)	0.72145(4)	0.7164(4)	-0.10159(4)	0.00692(11)
Te(4)	0.76483(4)	0.20708(4)	0.01113(4)	0.00670(11)
Te(5)	0.44335(4)	-0.04559(4)	0.38061(4)	0.00734(11)
Te(6)	-0.05734(4)	0.44296(4)	0.38305(4)	0.00744(11)
Ni(1)	0.96673(9)	0.61832(9)	0.00748(18)	0.00748(18)
Ni(2)	0.79809(9)	0.41108(9)	0.16836(8)	0.00817(18)
Ni(3)	0.42521(9)	0.78789(9)	0.17096(7)	0.00797(18)
Ni(4)	½	½	½	0.0066(2)
Ni(5)	0.24998(9)	0.55773(9)	0.25017(8)	0.00899(18)
Ni(6)	0.54480(9)	0.25936(9)	0.24556(8)	0.00967(19)
Ni(7)	0.62121(9)	-0.03322(9)	0.00734(18)	0.00734(18)
Ni(8)	0.26769(9)	0.26255(9)	0.46575(8)	0.00946(18)
Cl(1)	0.60835(18)	0.59434(18)	0.27183(15)	0.0142(3)
Cl(2)	0.21565(18)	0.76308(18)	0.33662(15)	0.0143(3)
Cl(3)	0.77090(19)	0.20744(19)	0.33189(15)	0.0168(3)
Cl(4)	0.4135(2)	0.4067(2)	0.39368(18)	0.0211(4)
Cl(5)	0.11152(18)	0.13897(18)	0.45624(17)	0.0169(4)
O(1)	0.0260(5)	0.0166(5)	-0.1342(4)	0.0113(10)
O(2)	0.7454(5)	0.0274(5)	-0.0820(4)	0.0099(9)
O(3)	0.0098(5)	0.7482(5)	-0.0831(10)	0.0113(10)
O(4)	0.0680(5)	0.6742(5)	0.1762(4)	0.0100(9)
O(5)	0.8013(5)	0.8049(5)	0.1416(4)	0.0108(9)
O(6)	0.8429(5)	0.5564(5)	0.0052(4)	0.0095(9)
O(7)	0.5719(5)	0.8292(5)	0.0092(4)	0.0102(9)
O(8)	0.6276(5)	0.6061(5)	-0.1301(4)	0.007(9)
O(9)	0.6623(5)	0.3691(5)	0.1013(4)	0.0088(9)
O(10)	0.6267(5)	0.3357(5)	-0.0995(4)	0.0075(9)
O(11)	0.6463(5)	0.1199(5)	0.1303(4)	0.0106(9)
O(12)	0.4681(5)	-0.0664(5)	0.2201(4)	0.0107(9)
O(13)	0.6347(5)	-0.0999(5)	0.4030(4)	0.0151(10)
O(14)	0.4080(5)	0.1553(5)	0.3327(4)	0.0109(9)
O(15)	0.1343(5)	0.4337(5)	0.3634(5)	0.0135(10)
O(16)	-0.0501(5)	0.4520(5)	0.2195(4)	0.0095(9)
O(17)	-0.1390(5)	0.6480(5)	0.3829(4)	0.0115(10)

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

Table S2 Selected Bond Lengths (Å) and Results from Bond Valence Sum (BVS) calculations for $Ni_{15}Te_{12}O_{34}Cl_{10}$.

Atom	Bond	Bond distance	Bond valence	Atom	Bond	Bond distance	Vond valence
Te(1)	Te(1)-O(1)	1.875(4)	1.4171	Te(4)	Te(4)-O(11)	1.889(4)	1.2685
	Te(1)-O(3)	1.891(5)	1.2617		Te(4)-O(9)	1.950(4)	1.0757
	Te(1)-O(2)	1.939(4)	1.1082		Te(4)-O(10)	1.959(4)	1.050
	Te(1)-Cl(3) #4	2.997(2)	0.1837		Te(4)-O(2) #3	2.497(4)	0.2453
	Te(1)-Cl(2) #7	3.076(2)	0.1836				3.64
			4.15				
				Te(5)	Te(5)-O(13)	1.872(5)	1.3281
Te(2)	Te(2)-O(5)	1.872(4)	1.3281		Te(5)-O(12)	1.875(4)	1.3174
	Te(2)-O(4)	1.927(4)	1.1447		Te(5)-O(14)	1.881(4)	1.2962
	Te(2)-O(17) #1	2.057(5)	0.8056				3.94
	Te(2)-O(1) #2	2.200(5)	0.5473				
			3.83	Te(6)	Te(6)-O(16)	1.862(5)	1.3645
					Te(6)-O(15)	1.889(5)	1.2685
Te(3)	Te(3)-O(8)	1.887(4)	1.2754		Te(6)-O(17)	1.897(4)	1.2414
	Te(3)-O(7)	1.901(4)	1.2280		Te(6)-Cl(5)	2.841(2)	0.2800
	Te(3)-O(6)	1.911(5)	1.1953				4.15
			3.70				
Ni(1)	Ni(1)-O(3)	2.046(5)	0.3466	Ni(5)	Ni(5)-O(4) #8	2.007(5)	0.3852
	Ni(1)-O(16) #1	2.053(5)	0.3401		Ni(5)-O(15)	2.085(5)	0.3120
	Ni(1)-O(4)	2.074(4)	0.3214		Ni(5)-O(10) #6	2.199(4)	0.2292
	Ni(1)-O(5)	2.080(4)	0.3162		Ni(5)-O(8) #6	2.200(4)	0.2286
	Ni(1)-O(6)	2.100(4)	0.2996		Ni(5)-Cl(4)	2.418(2)	0.3411
	Ni(1)-O(6) #4	2.194(4)	0.2324		Ni(5)-Cl(2)	2.4408(17)	0.3207
			1.86				1.82
Ni(2)	Ni(2)-O(9)	2.027(4)	0.3649	Ni(6)	Ni(6)-O(11)	1.980(4)	0.4143
	Ni(2)-O(16) #1	2.059(5)	0.3347		Ni(6)-O(14)	2.031(4)	0.3610
	Ni(2)-O(3) #4	2.128(5)	0.2777		Ni(6)-O(9)	2.145(4)	0.2653
	Ni(2)-O(6)	2.148(5)	0.2631		Ni(6)-O(8) #6	2.234(5)	0.2086
	Ni(2)-Cl(1)	2.349(2)	0.4110		Ni(6)-Cl(4)	2.3339(19)	0.4281
	Ni(2)-Cl(3)	2.473(2)	0.2940		Ni(6)-Cl(3)	2.577(2)	0.0825
			1.95				1.76
Ni(3)	Ni(3)-O(12) #5	2.000(4)	0.3925	Ni(7)	Ni(7)-O(11)	1.981(4)	0.4132
	Ni(3)-O(10) #6	2.015(4)	0.3769		Ni(7)-O(12)	2.013(4)	0.3790
	Ni(3)-O(7)	2.135(5)	0.2725		Ni(7)-O(5) #3	2.024(5)	0.3679
	Ni(3)-O(2) #7	2.175(5)	0.2446		Ni(7)-O(2) #3	2.060(5)	0.3338
	Ni(3)-Cl(1)	2.3469(19)	0.4133		Ni(7)-O(7) #3	2.106(4)	0.2948
	Ni(3)-Cl(2)	2.5210(18)	0.096		Ni(7)-O(7) #6	2.375(5)	0.1425
			1.80				1.93
Ni(4)	Ni(4)-O(10) #6	2.050(4)	0.3429	Ni(8)	Ni(8)-O(14)	2.000(5)	0.3925

	Ni(4)-O(10)	2.050(4)	0.3429
	Ni(4)-O(9) #6	2.054(5)	0.3392
	Ni(4)-O(9)	2.054(5)	0.3392
	Ni(4)-O(8)	2.116(4)	0.2869
	Ni(4)-O(8) #6	2.116(4)	0.2869
			1.94

O(1)	Te(1)-O(1)	1.875(4)	1.4171
	Te(2)-O(1) #2	2.200(5)	0.5473
			1.96

O(2)	Te(1)-O(2)	1.939(4)	1.1082
	Te(4)-O(2) #3	2.497(4)	0.2453
	Ni(3)-O(2) #7	2.175(5)	0.2446
	Ni(7)-O(2) #3	2.060(5)	0.3338
			1.93

O(3)	Te(1)-O(3)	1.891(5)	1.2617
	Ni(1)-O(3)	2.046(5)	0.3466
	Ni(2)-O(3) #4	2.128(5)	0.2777
			1.89

O(4)	Te(2)-O(4)	1.927(4)	1.1447
	Ni(1)-O(4)	2.074(4)	0.3214
	Ni(5)-O(4) #8	2.007(5)	0.3852
			1.85

O(5)	Te(2)-O(5)	1.872(4)	1.3281
	Ni(1)-O(5)	2.080(4)	0.3162
	Ni(7)-O(5) #3	2.024(5)	0.3679
			2.01

O(6)	Te(3)-O(6)	1.911(5)	1.1953
	Ni(1)-O(6)	2.100(4)	0.2996
	Ni(1)-O(6) #4	2.194(4)	0.2324
	Ni(2)-O(6)	2.148(5)	0.2631
			1.99

O(7)	Te(3)-O(7)	1.901(4)	1.2280
	Ni(3)-O(7)	2.135(5)	0.2725
	Ni(7)-O(7) #3	2.106(4)	0.2948
	Ni(7)-O(7) #6	2.375(5)	0.1425
			1.94

	Ni(8)-O(15)	2.002(5)	0.3904
	Ni(8)-O(13) #9	2.022(5)	0.3699
	Ni(8)-O(17) #10	2.058(4)	0.3356
	Ni(8)-Cl(4)	2.4041(19)	0.3541
	Ni(8)-Cl(5)	2.5007(18)	0.1014
			1.94

O(10)	Te(4)-O(10)	1.959(4)	1.050
	Ni(3)-O(10) #6	2.015(4)	0.3769
	Ni(4)-O(10)	2.050(4)	0.3429
	Ni(5)-O(10) #6	2.199(4)	0.2292
			2.00

O(11)	Te(4)-O(11)	1.889(4)	1.2685
	Ni(6)-O(11)	1.980(4)	0.4143
	Ni(7)-O(11)	1.981(4)	0.4132
			2.09

O(12)	Te(5)-O(12)	1.875(4)	1.3174
	Ni(3)-O(12) #5	2.000(4)	0.3925
	Ni(7)-O(12)	2.013(4)	0.3790
			2.09

O(13)	Te(5)-O(13)	1.872(5)	1.3281
	Ni(8)-O(13) #9	2.022(5)	0.3699
			1.70

O(14)	Te(5)-O(14)	1.881(4)	1.2962
	Ni(6)-O(14)	2.031(4)	0.3610
	Ni(8)-O(14)	2.000(5)	0.3925
			2.05

O(15)	Te(6)-O(15)	1.889(5)	1.2685
	Ni(5)-O(15)	2.085(5)	0.3120
	Ni(8)-O(15)	2.002(5)	0.3904
			1.97

O(16)	Te(6)-O(16)	1.862(5)	1.3645
	Ni(1)-O(16) #1	2.053(5)	0.3401
	Ni(2)-O(16) #1	2.059(5)	0.3347
			2.04

O(8)	Te(3)-O(8)	1.887(4)	1.2754
	Ni(4)-O(8)	2.116(4)	0.2869
	Ni(5)-O(8) #6	2.200(4)	0.2286
	Ni(6)-O(8) #6	2.234(5)	0.2086
			2.00
O(9)	Te(4)-O(9)	1.950(4)	1.0757
	Ni(2)-O(9)	2.027(4)	0.3649
	Ni(4)-O(9)	2.054(5)	0.3392
	Ni(6)-O(9)	2.145(4)	0.2653
			2.05
Cl(1)	Ni(2)-Cl(1)	2.349(2)	0.4110
	Ni(3)-Cl(1)	2.3469(19)	0.4133
			0.83
Cl(2)	Te(1)-Cl(2) #7	3.076(2)	0.1836
	Ni(3)-Cl(2)	2.5210(18)	0.096
	Ni(5)-Cl(2)	2.4408(17)	0.3207
			0.60
Cl(3)	Te(1)-Cl(3) #4	2.997(2)	0.1837
	Ni(2)-Cl(3)	2.473(2)	0.2940
	Ni(6)-Cl(3)	2.577(2)	0.0825
			0.56
O(17)	Te(2)-O(17) #1	2.057(5)	0.8056
	Te(6)-O(17)	1.897(4)	1.2414
	Ni(8)-O(17) #10	2.058(4)	0.3356
			2.38
Cl(4)	Ni(5)-Cl(4)	2.418(2)	0.3411
	Ni(6)-Cl(4)	2.3339(19)	0.4281
	Ni(8)-Cl(4)	2.4041(19)	0.3541
			1.12
Cl(5)	Te(6)-Cl(5)	2.841(2)	0.2800
	Ni(8)-Cl(5)	2.5007(18)	0.1014
			0.38

Note. Symmetry transformations used to generate equivalent atoms:

#1 1+x, y, z	#2 2-x, 2-y, -z	#3 x, y-1, z	#4 -x+2, 1-y, -z
#5 x, y+1, z	#6 -x+1, 1-y, -z	#7 1-x, 2-y, -z	#8 x-1, y, z
#9 1-x, -y, 1-z	#10 -x, 1-y, 1-z		

Bond valence sum (BVS) calculations according to Brown and Altermatt [A].

The r_0 values used are Te-O: 1.977, Te-Cl: 2.37, Ni-O: 1.654, Ni-Cl: 2.02 [B]

Table S3 Selected Bond Angles (°) for $Ni_{15}Te_{12}O_{34}Cl_{10}$.

O(1)-Te(1)-O(3)	93.3(2)	O(2)#7-Ni(3)-Cl(2)	85.2(1)
O(1)-Te(1)-O(2)	92.1(2)	Cl(1)-Ni(3)-Cl(2)	94.4(6)
O(3)-Te(1)-O(2)	101.1(2)	O(10)#6-Ni(4)-O(10)	180.0(2)
O(1)-Te(1)-Cl(3) #4	82.36(16)	O(10)-Ni(4)-O(9) #6	101.4(2)
O(3)-Te(1)-Cl(3) #4	78.31(16)	O(10)-Ni(4)-O(9)	78.6(2)
O(2)-Te(1)-Cl(3) #4	174.28(16)	O(10)#6-Ni(4)-O(9) #6	78.6(2)
O(1)-Te(1)-Cl(2) #7	86.08(17)	O(10)#6-Ni(4)-O(9)	101.4(2)
O(3)-Te(1)-Cl(2) #7	176.13(16)	O(9)#6-Ni(4)-O(9)	180.0(3)
O(2)-Te(1)-Cl(2) #7	75.21(16)	O(10)#6-Ni(4)-O(8)	98.6(2)
Cl(3)#4-Te(1)-Cl(2) #7	105.40(5)	O(10)-Ni(4)-O(8)	81.4(2)
O(5)-Te(2)-O(4)	84.9(2)	O(9)-Ni(4)-O(8)	95.0(2)
O(5)-Te(2)-O(17) #1	95.2(2)	O(9)#6-Ni(4)-O(8)	85.0(2)
O(4)-Te(2)-O(17) #1	88.2(2)	O(10)#6-Ni(4)-O(8) #6	81.4(2)
O(5)-Te(2)-O(1) #2	97.0(2)	O(10)-Ni(4)-O(8) #6	98.6(2)
O(4)-Te(2)-O(1) #2	86.3(2)	O(9)-Ni(4)-O(8) #6	85.0(2)
O(17)#3-Te(2)-O(1) #2	166.2(2)	O(9)#6-Ni(4)-O(8) #6	95.0(2)
O(8)-Te(3)-O(7)	101.9(2)	O(8)-Ni(4)-O(8) #6	180.0(2)
O(8)-Te(3)-O(6)	97.7(2)	O(4)#8-Ni(5)-O(15)	85.3(2)
O(7)-Te(3)-O(6)	101.7(2)	O(4)#8-Ni(5)-O(10) #6	90.5(2)
O(11)-Te(4)-O(9)	84.2(2)	O(15)-Ni(5)-O(10) #6	167.2(2)
O(11)-Te(4)-O(10)	100.3(2)	O(4)#8-Ni(5)-O(8) #6	99.7(2)
O(9)-Te(4)-O(10)	83.4(2)	O(15)-Ni(5)-O(8) #6	92.5(2)
O(11)-Te(4)-O(2) #3	73.4(2)	O(10)#6-Ni(5)-O(8) #6	76.3(2)
O(9)-Te(4)-O(2) #3	147.2(2)	O(4)#8-Ni(5)-Cl(4)	162.2(1)
O(10)-Te(4)-O(2) #3	77.6(2)	O(15)-Ni(5)-Cl(4)	79.2(1)
O(13)-Te(5)-O(12)	104.1(2)	O(10)#6-Ni(5)-Cl(4)	106.5(1)
O(13)-Te(5)-O(14)	93.4(2)	O(8)#6-Ni(5)-Cl(4)	89.7(1)
O(12)-Te(5)-O(14)	92.0(2)	O(4)#8-Ni(5)-Cl(2)	92.7(1)
O(16)-Te(6)-O(15)	95.9(2)	O(15)-Ni(5)-Cl(2)	112.3(2)
O(16)-Te(6)-O(17)	98.2(2)	O(10)#6-Ni(5)-Cl(2)	79.8(1)
O(15)-Te(6)-O(17)	90.8(2)	O(8)#6-Ni(5)-Cl(2)	153.1(1)
O(16)-Te(6)-Cl(5)	101.3(2)	Cl(4)-Ni(5)-Cl(2)	85.3(7)
O(15)-Te(6)-Cl(5)	76.5(2)	O(11)-Ni(6)-O(14)	91.0(2)
O(17)-Te(6)-Cl(5)	157.70(2)	O(11)-Ni(6)-O(9)	77.1(2)
O(3)-Ni(1)-O(16) #1	167.7(2)	O(14)-Ni(6)-O(9)	160.2(2)
O(3)-Ni(1)-O(4)	96.1(2)	O(11)-Ni(6)-O(8) #6	89.7(2)
O(16)#1-Ni(1)-O(4)	90.0(2)	O(14)-Ni(6)-O(8) #6	84.2(2)
O(3)-Ni(1)-O(5)	89.3(2)	O(9)-Ni(6)-O(8) #6	80.1(2)
O(16)#1-Ni(1)-O(5)	102.6(2)	O(11)-Ni(6)-Cl(4)	173.9(1)
O(4)-Ni(1)-O(5)	76.2(2)	O(14)-Ni(6)-Cl(4)	83.1(1)
O(3)-Ni(1)-O(6)	91.8(2)	O(9)-Ni(6)-Cl(4)	109.0(1)
O(16)#1-Ni(1)-O(6)	83.1(2)	O(8)#6-Ni(6)-Cl(4)	91.0(1)
O(4)-Ni(1)-O(6)	171.0(2)	O(11)-Ni(6)-Cl(3)	97.5(2)
O(5)-Ni(1)-O(6)	99.7(2	O(14)-Ni(6)-Cl(3)	120.7(1)
O(3)-Ni(1)-O(6) #4	83.2(2)	O(9)-Ni(6)-Cl(3)	77.0(1)
O(16)#1-Ni(1)-O(6) #4	85.2(2)	O(8)#6-Ni(6)-Cl(3)	153.7(1)
O(4)-Ni(1)-O(6) #4	100.4(2)	Cl(4)-Ni(6)-Cl(3)	84.5(6)
O(5)-Ni(1)-O(6) #4	171.4(2)	O(11)-Ni(7)-O(12)	98.4(2)
O(6)-Ni(1)-O(6) #4	84.8(2)	O(11)-Ni(7)-O(5) #3	92.6(2)

O(9)-Ni(2)-O(16) #1	174.2(2)	O(12)-Ni(7)-O(5) #3	98.0(2)
O(9)-Ni(2)-O(3) #4	92.8(2)	O(11)-Ni(7)-O(2) #3	82.5(2)
O(16)#1-Ni(2)-O(3) #4	82.8(2)	O(12)-Ni(7)-O(2) #3	169.5(2)
O(9)-Ni(2)-O(6)	93.9(2)	O(5)#3-Ni(7)-O(2) #3	92.5(2)
O(16)#1-Ni(2)-O(6)	81.8(2)	O(11)-Ni(7)-O(7) #3	171.8(2)
O(3)#4-Ni(2)-O(6)	82.5(2)	O(12)-Ni(7)-O(7) #3	82.1(2)
O(9)-Ni(2)-Cl(1)	95.1(1)	O(5)#3-Ni(7)-O(7) #3	95.4(2)
O(16)#1-Ni(2)-Cl(1)	89.3(1)	O(2)#3-Ni(7)-O(7) #3	95.6(2)
O(3)#4-Ni(2)-Cl(1)	172.1(1)	O(11)-Ni(7)-O(7) #6	83.5(2)
O(6)-Ni(2)-Cl(1)	96.6(1)	O(12)-Ni(7)-O(7) #6	88.0(2)
O(9)-Ni(2)-Cl(3)	81.6(1)	O(5)#3-Ni(7)-O(7) #6	173.4(2)
O(16)#1-Ni(2)-Cl(3)	101.9(1)	O(2)#3-Ni(7)-O(7) #6	81.7(2)
O(3)#4-Ni(2)-Cl(3)	87.9(1)	O(7)#3-Ni(7)-O(7) #6	88.3(2)
O(6)-Ni(2)-Cl(3)	169.1(1)	O(14)-Ni(8)-O(15)	98.1(2)
Cl(1)-Ni(2)-Cl(3)	93.6(6)	O(14)-Ni(8)-O(13) #9	92.8(2)
O(12)#5-Ni(3)-O(10) #6	171.4(2)	O(15)-Ni(8)-O(13) #9	168.1(2)
O(12)#5-Ni(3)-O(7)	81.6(2)	O(14)-Ni(8)-O(17) #10	172.9(2)
O(10)#6-Ni(3)-O(7)	93.3(2)	O(15)-Ni(8)-O(17) #10	89.0(2)
O(12)#5-Ni(3)-O(2) #7	88.0(2)	O(13)#9-Ni(8)-O(17) #10	80.2(2)
O(10)#6-Ni(3)-O(2) #7	84.6(2)	O(14)-Ni(8)-Cl(4)	81.9(1)
O(7)-Ni(3)-O(2) #7	84.9(2)	O(15)-Ni(8)-Cl(4)	81.2(1)
O(12)#5-Ni(3)-Cl(1)	90.0(1)	O(13)#9-Ni(8)-Cl(4)	105.4(2)
O(10)#6-Ni(3)-Cl(1)	97.4(1)	O(17)#10-Ni(8)-Cl(4)	99.3(1)
O(7)-Ni(3)-Cl(1)	95.7(1)	O(14)-Ni(8)-Cl(5)	84.7(1)
O(2)#7-Ni(3)-Cl(1)	177.8(1)	O(15)-Ni(8)-Cl(5)	83.6(1)
O(12)#5-Ni(3)-Cl(2)	102.4(1)	O(13)#9-Ni(8)-Cl(5)	92.6(2)
O(10)#6-Ni(3)-Cl(2)	81.4(1)	O(17)#10-Ni(8)-Cl(5)	96.1(1)
O(7)-Ni(3)-Cl(2)	169.2(1)	Cl(4)-Ni(8)-Cl(5)	158.0(7)

Note. Symmetry transformations used to generate equivalent atoms:

#1 1+x, y, z	#2 2-x, 2-y, -z	#3 x, y-1, z	#4 -x+2, 1-y, -z
#5 x, y+1, z	#6 -x+1, 1-y, -z	#7 1-x, 2-y, -z	#8 x-1, y, z
#9 1-x, -y, 1-z	#10 -x, 1-y, 1-z		

References

[A] I.D. Brown, D. Altermatt, *Acta Cryst.*, 1985, **B41**, 244–247.

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