Supporting Information

$BaCa_2M_6Te_3O_{18}$ (M = Co, Ni): New 1D zigzag spin-chain compounds with a stacked kagomé structure

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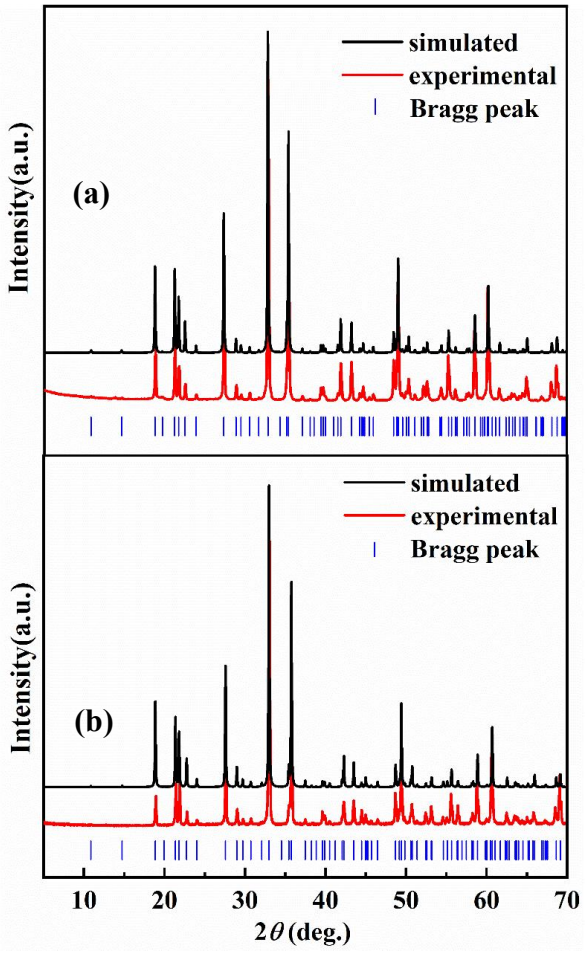

Figure S1. Experimental and calculated XRD patterns of (a) $BaCa_2Co_6Te_3O_{18}$ and (b) $BaCa_2Ni_6Te_3O_{18}$.

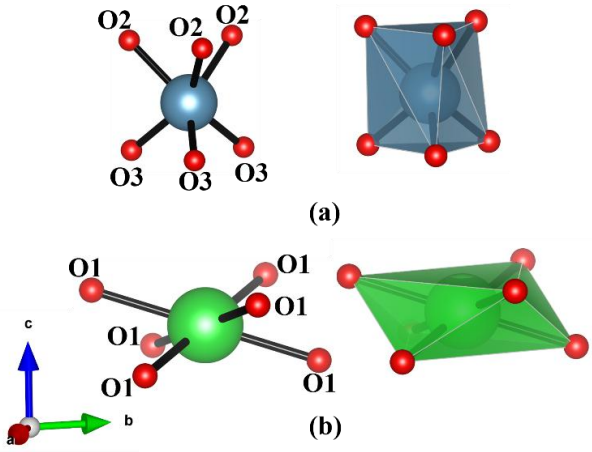

Figure S2. View of the oxygen-coordination environments for (a) Ca and (b) Ba atoms in $BaCa_2M_6Te_3O_{18}$ (M = Co, Ni).

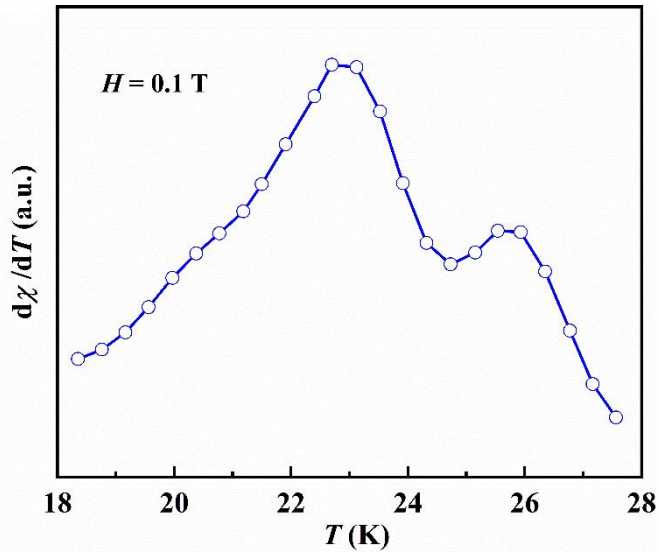

Figure S3. The derivative of magnetic susceptibility for $BaCa_2Ni_6Te_3O_{18}$.

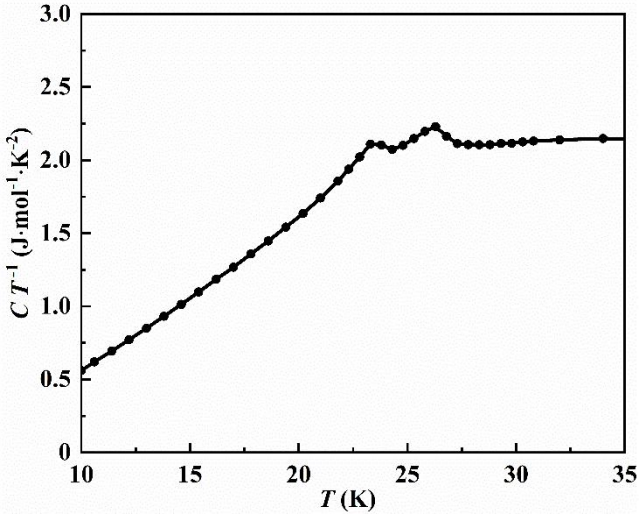

Figure S4. An enlarged view of low-temperature heat capacity data for $BaCa_2Ni_6Te_3O_{18}$.

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $BaCa_2M_6Te_3O_{18}$ (M = Co, Ni). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Ba1	0	10000	5000	5.4(3)
Te1	133.5(7)	6560.3(7)	2500	2.3(2)
Co1	3536.5(12)	10000.6(11)	4088.4(10)	3.5(3)
Ca1	3333.33	6666.67	5612(2)	3.2(5)
O1	-1144(6)	6790(6)	4067(5)	6.9(10)
O2	-1289(8)	4191(8)	2500	4.8(13)
O3	1220(6)	6097(6)	4072(5)	6.5(10)
O4	1697(8)	8889(8)	2500	7.0(14)
Atom	**x**	**y**	**z**	**U(eq)**
Ba1	0	0	0	4.39(18)
Te1	3614.3(5)	3417.8(4)	2500	1.17(16)
Ni1	3517.1(7)	-69.1(7)	895.3(6)	3.09(19)
Ca1	6666.67	3333.33	5622.2(18)	6.2(3)
O1	2094(4)	3183(4)	921(3)	3.5(6)
O2	4570(5)	5838(5)	2500	3.7(8)
O3	5168(3)	3921(3)	4097(3)	2.7(6)
O4	2867(5)	1101(5)	2500	4.4(8)

Table S2. Anisotropic displacement parameters of $BaCa_2M_6Te_3O_{18}$ (M = Co, Ni). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Ba1	2.7(3)	2.7(3)	10.7(5)	0	0	1.35(16)
Te1	2.5(3)	1.8(3)	2.4(3)	0	0	0.9(3)
Co1	3.1(5)	4.2(5)	3.7(5)	-0.5(3)	0.0(3)	2.1(4)
Ca1	3.4(7)	3.4(7)	2.8(10)	0	0	1.7(3)
O1	8(3)	12(3)	4(2)	-0.4(18)	1.6(17)	8(2)
O2	5.0(16)	4.3(16)	5.5(16)	0	0	2.6(11)
O3	6.6(13)	6.5(13)	6.5(13)	0.3(9)	0.0(9)	3.4(9)
O4	6(3)	5(3)	8(3)	0	0	1(3)
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Ba1	2.2(2)	2.2(2)	8.7(4)	0	0	1.12(10)
Te1	1.3(2)	0.9(2)	1.1(3)	0	0	0.39(14)
Ni1	2.9(3)	3.9(3)	3.0(4)	-0.15(19)	-0.22(18)	2.1(2)
Ca1	5.9(4)	5.9(4)	6.7(8)	0	0	3.0(2)
O1	2.1(13)	6.3(14)	1.8(16)	0.9(11)	0.1(11)	1.9(12)
O2	4.3(11)	2.7(11)	4.0(12)	0	0	1.7(9)
O3	2.3(9)	3.3(9)	1.5(10)	0.3(7)	0.2(7)	0.7(7)
O4	6.4(19)	3.6(19)	3(2)	0	0	2.2(16)

Table S3. Selected bond lengths [Å] for $BaCa_2Co_6Te_3O_{18}$.

Atom-Atom	Length/Å	Atom-Atom	Length/Å
Ba1-O1	2.793(5)	Te1-O4	1.943(7)
Ba1-O1[1]	2.793(5)	Co1-O1[4]	2.090(5)
Ba1-O1[2]	2.793(5)	Co1-O1[3]	2.123(5)
Ba1-O1[3]	2.793(5)	Co1-O2[11]	2.161(5)
Ba1-O1[4]	2.793(5)	Co1-O3[4]	2.145(5)
Ba1-O1[5]	2.793(5)	Co1-O3[11]	2.097(5)
Ba1-O4[4]	3.231(5)	Co1-O4	2.086(5)
Ba1-O4[3]	3.231(5)	Ca1-O1[4]	2.877(5)
Ba1-O4[1]	3.231(5)	Ca1-O1[12]	2.877(5)
Ba1-O4[5]	3.231(5)	Ca1-O1[7]	2.877(5)
Ba1-O4[2]	3.231(5)	Ca1-O2[12]	2.392(5)
Ba1-O4	3.231(5)	Ca1-O2[4]	2.392(5)
Te1-O1	1.940(5)	Ca1-O2[7]	2.392(5)
Te1-O1[9]	1.940(5)	Ca1-O3	2.266(5)
Te1-O2	1.952(7)	Ca1-O3[11]	2.266(5)
Te1-O3	1.925(5)	Ca1-O3[13]	2.266(5)
Te1-O3[9]	1.925(5)		

Symmetry transformations used to generate equivalent atoms:

[1]-X,2-Y,1-Z; [2]-1+Y,-X+Y,1-Z; [3]1-Y,2+X-Y,+Z; [4]1-Y+X,1+X,1-Z; [5]-1+Y-X,1-X,+Z; [6]-1+Y,-X+Y,-1/2+Z; [7]-X,1-Y,1-Z; [8]-X,1-Y,-1/2+Z; [9]+X,+Y,1/2-Z; [10]1-X,2-Y,1-Z; [11]+Y-X,1-X,+Z; [12]+Y,-X+Y,1-Z; [13]1-Y,1+X-Y,+Z

Table S4. Selected bond angles for $BaCa_2Co_6Te_3O_{18}$.

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O1-Ba1-O1[1]	164.3(2)	O1[10]-Te1-O1	93.5(3)
O1-Ba1-O1[2]	87.5(2)	O1[10]-Te1-O2	91.0(2)
O1[1]-Ba1-O1[3]	89.3(3)	O1-Te1-O2	91.0(2)
O1[1]-Ba1-O1[4]	78.4(2)	O1[10]-Te1-O4	92.1(2)
O1[1]-Ba1-O1[5]	180	O1-Te1-O4	92.1(2)
O1-Ba1-O1[3]	111.33(9)	O3-Te1-O1[10]	174.0(2)
O1[5]-Ba1-O1[3]	111.33(9)	O3[10]-Te1-O1	174.0(2)
O1[4]-Ba1-O1[3]	68.67(9)	O3-Te1-O1	85.5(2)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
$O1^{1}$-Ba1-$O1^{2}$	111.33(9)	$O3^{10}$-Te1-$O1^{10}$	85.5(2)
$O1^{5}$-Ba1-$O1^{4}$	68.67(9)	$O3^{10}$-Te1-O2	83.0(2)
$O1^{5}$-Ba1-$O1^{2}$	111.33(9)	O3-Te1-O2	83.0(2)
$O1^{4}$-Ba1-$O1^{2}$	68.67(9)	O3-Te1-$O3^{10}$	94.8(3)
O1-Ba1-$O1^{4}$	68.67(9)	O3-Te1-O4	93.9(2)
O1-Ba1-$O1^{5}$	180	$O3^{10}$-Te1-O4	93.9(2)
$O1^{3}$-Ba1-$O1^{2}$	68.67(9)	O4-Te1-O2	175.4(3)
$O1^{4}$-Ba1-$O4^{2}$	111.33(9)	$O1^{3}$-Co1-$O1^{4}$	96.8(2)
$O1^{4}$-Ba1-$O4^{3}$	111.33(9)	$O1^{4}$-Co1-$O2^{12}$	87.1(2)
O1-Ba1-$O4^{3}$	68.67(9)	$O1^{3}$-Co1-$O2^{12}$	167.74(19)
$O1^{5}$-Ba1-$O4^{4}$	180	$O1^{3}$-Co1-$O3^{3}$	76.54(18)
$O1^{2}$-Ba1-O4	118.16(13)	$O1^{3}$-Co1-$O3^{12}$	98.58(19)
O1-Ba1-$O4^{2}$	61.84(13)	$O1^{4}$-Co1-$O3^{3}$	84.09(19)
$O1^{4}$-Ba1-$O4^{1}$	121.68(15)	$O3^{12}$-Co1-$O1^{4}$	155.7(2)
$O1^{5}$-Ba1-$O4^{5}$	125.29(15)	$O3^{3}$-Co1-$O2^{12}$	92.37(18)
$O1^{3}$-Ba1-O4	118.16(13)	$O3^{12}$-Co1-$O2^{12}$	74.2(2)
$O1^{2}$-Ba1-$O4^{3}$	58.32(15)	$O3^{12}$-Co1-$O3^{3}$	81.3(2)
$O1^{1}$-Ba1-$O4^{1}$	121.68(15)	O4-Co1-$O1^{3}$	96.62(19)
$O1^{5}$-Ba1-$O4^{1}$	54.71(15)	O4-Co1-$O1^{4}$	89.4(2)
$O1^{5}$-Ba1-$O4^{2}$	61.84(13)	O4-Co1-$O2^{12}$	95.04(18)
$O1^{2}$-Ba1-$O4^{5}$	125.29(15)	O4-Co1-$O3^{12}$	107.4(2)
$O1^{3}$-Ba1-$O4^{1}$	54.71(15)	O4-Co1-$O3^{3}$	169.9(2)
$O1^{3}$-Ba1-$O4^{2}$	58.32(15)	$O1^{8}$-Ca1-$O1^{14}$	119.00(3)
O1-Ba1-O4	61.84(13)	$O1^{3}$-Ca1-$O1^{8}$	119.00(4)
$O1^{5}$-Ba1-$O4^{3}$	121.68(15)	$O1^{3}$-Ca1-$O1^{14}$	119.00(4)
$O1^{3}$-Ba1-$O4^{4}$	118.16(13)	$O2^{8}$-Ca1-$O1^{14}$	128.75(17)
$O1^{1}$-Ba1-$O4^{2}$	125.29(15)	$O2^{8}$-Ca1-$O1^{8}$	62.81(19)
$O1^{4}$-Ba1-$O4^{5}$	54.71(15)	$O2^{14}$-Ca1-$O1^{3}$	128.75(17)
$O1^{3}$-Ba1-$O4^{5}$	118.16(13)	$O2^{3}$-Ca1-$O1^{14}$	67.42(19)
$O1^{1}$-Ba1-O4	121.68(15)	$O2^{8}$-Ca1-$O1^{3}$	67.42(19)
$O1^{1}$-Ba1-$O4^{4}$	121.68(15)	$O2^{14}$-Ca1-$O1^{14}$	62.81(19)
$O1^{1}$-Ba1-$O4^{5}$	125.29(15)	$O2^{3}$-Ca1-$O1^{3}$	62.81(19)
$O1^{4}$-Ba1-$O4^{4}$	58.32(15)	$O2^{3}$-Ca1-$O1^{8}$	128.75(17)
$O1^{5}$-Ba1-O4	125.29(16)	$O2^{14}$-Ca1-$O1^{8}$	67.42(19)
$O1^{2}$-Ba1-$O4^{4}$	61.84(13)	$O2^{3}$-Ca1-$O2^{8}$	74.94(19)
$O1^{1}$-Ba1-$O4^{3}$	118.16(13)	$O2^{8}$-Ca1-$O2^{14}$	74.94(19)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O1-Ba1-O4^{4}	54.71(15)	O2^{3}-Ca1-O2^{14}	74.94(19)
O1-Ba1-O4^{5}	121.68(15)	O3^{15}-Ca1-O1^{8}	66.32(16)
O1^{4}-Ba1-O4	58.32(15)	O3^{15}-Ca1-O1^{14}	75.16(16)
O1^{2}-Ba1-O4^{1}	58.32(15)	O3-Ca1-O1^{3}	66.32(15)
O1^{2}-Ba1-O4^{2}	118.16(13)	O3-Ca1-O1^{8}	75.16(16)
O1^{3}-Ba1-O4^{3}	61.84(13)	O3^{15}-Ca1-O1^{3}	147.46(17)
O1-Ba1-O4^{1}	58.32(15)	O3-Ca1-O1^{14}	147.46(17)
O4-Ba1-O4^{5}	61.84(13)	O3^{12}-Ca1-O1^{8}	147.46(17)
O4^{2}-Ba1-O4^{4}	54.71(15)	O3^{12}-Ca1-O1^{14}	66.32(15)
O4^{1}-Ba1-O4^{5}	54.71(15)	O3^{12}-Ca1-O1^{3}	75.16(16)
O4-Ba1-O4^{3}	125.29(15)	O3^{12}-Ca1-O2^{14}	129.0(2)
O4^{3}-Ba1-O4^{1}	103.33(14)	O3-Ca1-O2^{14}	142.2(2)
O4-Ba1-O4^{1}	76.67(14)	O3-Ca1-O2^{3}	129.0(2)
O4-Ba1-O4^{4}	76.67(14)	O3^{15}-Ca1-O2^{8}	129.0(2)
O4^{3}-Ba1-O4^{4}	103.33(14)	O3^{15}-Ca1-O2^{3}	142.2(2)
O4^{1}-Ba1-O4^{4}	76.67(14)	O3^{15}-Ca1-O2^{14}	83.66(17)
O4^{2}-Ba1-O4^{1}	180.0(4)	O3-Ca1-O2^{8}	83.66(17)
O4-Ba1-O4^{2}	76.67(14)	O3^{12}-Ca1-O2^{3}	83.66(17)
O4^{3}-Ba1-O4^{2}	103.33(14)	O3^{12}-Ca1-O2^{8}	142.2(2)
O4^{2}-Ba1-O4^{5}	103.33(14)	O3^{12}-Ca1-O3^{15}	86.31(18)
O4^{3}-Ba1-O4^{5}	103.33(14)	O3-Ca1-O3^{15}	86.31(18)
O4^{5}-Ba1-O4^{4}	76.67(14)	O3-Ca1-O3^{12}	86.31(18)

Symmetry transformations used to generate equivalent atoms:

^{1}-X,2-Y,1-Z; ^{2}-1+Y-X,1-X,+Z; ^{3}1-Y+X,1+X,1-Z; ^{4}1-Y,2+X-Y,+Z; ^{5}-1+Y,-X+Y,1-Z; ^{6}-X,2-Y,-1/2+Z; ^{7}-1+Y,-X+Y,-1/2+Z; ^{8}-X,1-Y,1-Z; ^{9}-X,1-Y,-1/2+Z; ^{10}+X,+Y,1/2-Z; ^{11}1-X,2-Y,1-Z; ^{12}+Y-X,1-X,+Z; ^{13}1-Y+X,+X,1-Z; ^{14}+Y,-X+Y,1-Z; ^{15}1-Y,1+X-Y,+Z; ^{16}1-Y,1+X-Y,1/2-Z

Table S5. Selected bond lengths [Å] for $BaCa_2Ni_6Te_3O_{18}$.

Atom-Atom	Length/Å	Atom-Atom	Length/Å
Ba1-O1	2.759(3)	Te1-O4	1.926(4)
Ba1-O1[1]	2.759(3)	Ni1-O1[5]	2.119(3)
Ba1-O1[2]	2.759(3)	Ni1-O1[3]	2.059(3)
Ba1-O1[3]	2.759(3)	Ni1-O2[13]	2.089(3)
Ba1-O1[4]	2.759(3)	Ni1-O3[14]	2.086(3)
Ba1-O1[5]	2.759(3)	Ni1-O3[15]	2.086(3)
Ba1-O4[3]	3.240(3)	Ni1-O4	2.073(3)
Ba1-O4	3.240(3)	Ca1-O1[16]	2.888(3)
Ba1-O4[5]	3.240(3)	Ca1-O1[17]	2.888(3)
Ba1-O4[1]	3.240(3)	Ca1-O1[18]	2.888(3)
Ba1-O4[2]	3.240(3)	Ca1-O2[19]	2.378(3)
Ba1-O4[4]	3.240(3)	Ca1-O2[20]	2.378(3)
Te1-O1	1.937(3)	Ca1-O2[9]	2.378(3)
Te1-O1[11]	1.937(3)	Ca1-O3[13]	2.216(3)
Te1-O2	1.986(4)	Ca1-O3	2.216(3)
Te1-O3[11]	1.921(3)	Ca1-O3[7]	2.216(3)
Te1-O3	1.921(3)		

Symmetry transformations used to generate equivalent atoms:

1-Y,+X-Y,+Z; [2]-Y+X,+X,-Z; [3]+Y,-X+Y,-Z; [4]-X,-Y,-Z; [5]+Y-X,-X,+Z; [6]-Y+X,+X,1/2+Z; [7]1+Y-X,1-X,+Z; [8]1+Y-X,1-X,1/2-Z; [9]1-X,1-Y,1-Z; [10]1-X,1-Y,-1/2+Z; [11]+X,+Y,1/2-Z; [12]1-X,-Y,-1/2+Z; [13]1-Y,+X-Y,+Z; [14]+Y,-X+Y,-1/2+Z; [15]1-Y,+X-Y,1/2-Z; [16]1-Y+X,+X,1/2+Z; [17]1-X,1-Y,1/2+Z; [18]+Y,-X+Y,1/2+Z; [19]1-Y+X,+X,1-Z; [20]+Y,-X+Y,1-Z

Table S6. Selected bond angles for $BaCa_2Ni_6Te_3O_{18}$.

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O1-Ba1-O1[1]	180	O1[11]-Te1-O1	93.03(17)
O1[1]-Ba1-O1[2]	68.44(5)	O1-Te1-O2	90.91(12)
O1-Ba1-O1[3]	68.44(5)	O1[11]-Te1-O2	90.91(12)
O1[2]-Ba1-O1[3]	68.44(5)	O3[11]-Te1-O1	85.30(12)
O1[4]-Ba1-O1[2]	180	O3[11]-Te1-O1[11]	172.93(12)
O1[2]-Ba1-O1[5]	111.56(5)	O3-Te1-O1[11]	85.30(12)
O1-Ba1-O1[4]	68.44(5)	O3-Te1-O1	172.93(12)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
$O1^{4}$-Ba1-$O1^{3}$	111.56(5)	$O3^{11}$-Te1-O2	82.25(12)
O1-Ba1-$O1^{5}$	111.56(5)	O3-Te1-O2	82.25(12)
$O1^{1}$-Ba1-$O1^{5}$	68.44(5)	$O3^{11}$-Te1-O3	95.52(17)
$O1^{1}$-Ba1-$O1^{4}$	111.56(5)	$O3^{11}$-Te1-O4	94.65(12)
$O1^{4}$-Ba1-$O1^{5}$	68.44(5)	O3-Te1-O4	94.65(12)
$O1^{1}$-Ba1-$O1^{3}$	111.56(5)	O4-Te1-O1	92.28(12)
O1-Ba1-$O1^{2}$	111.56(5)	O4-Te1-$O1^{11}$	92.28(12)
$O1^{3}$-Ba1-$O1^{5}$	180.00(10)	O4-Te1-O2	175.36(16)
O1-Ba1-$O4^{4}$	121.50(9)	$O1^{4}$-Ni1-$O1^{5}$	95.90(14)
$O1^{3}$-Ba1-$O4^{1}$	58.50(9)	$O1^{4}$-Ni1-$O2^{12}$	169.93(12)
$O1^{3}$-Ba1-$O4^{5}$	125.38(8)	$O1^{4}$-Ni1-$O3^{14}$	97.18(11)
$O1^{1}$-Ba1-$O4^{4}$	58.50(9)	$O1^{4}$-Ni1-$O3^{15}$	78.17(11)
$O1^{4}$-Ba1-$O4^{5}$	121.50(9)	$O1^{4}$-Ni1-O4	95.56(12)
$O1^{4}$-Ba1-$O4^{4}$	54.62(8)	$O2^{12}$-Ni1-$O1^{5}$	88.89(13)
$O1^{1}$-Ba1-$O4^{2}$	121.50(9)	$O3^{14}$-Ni1-$O1^{5}$	159.82(11)
$O1^{2}$-Ba1-$O4^{4}$	125.38(8)	$O3^{15}$-Ni1-$O1^{5}$	86.08(11)
O1-Ba1-$O4^{5}$	119.28(8)	$O3^{14}$-Ni1-$O2^{12}$	75.98(13)
$O1^{2}$-Ba1-$O4^{5}$	58.50(9)	$O3^{15}$-Ni1-$O2^{12}$	93.38(11)
$O1^{5}$-Ba1-$O4^{4}$	60.72(8)	$O3^{15}$-Ni1-$O3^{14}$	81.65(12)
$O1^{4}$-Ba1-$O4^{3}$	58.50(9)	O4-Ni1-$O1^{5}$	89.88(14)
O1-Ba1-$O4^{2}$	58.50(9)	O4-Ni1-$O2^{12}$	93.29(11)
$O1^{4}$-Ba1-O4	60.72(8)	O4-Ni1-$O3^{14}$	104.04(14)
$O1^{3}$-Ba1-$O4^{3}$	54.62(8)	O4-Ni1-$O3^{15}$	172.13(12)
$O1^{2}$-Ba1-O4	119.28(8)	$O1^{18}$-Ca1-$O1^{20}$	119.16(2)
$O1^{5}$-Ba1-O4	58.50(9)	$O1^{19}$-Ca1-$O1^{20}$	119.16(2)
$O1^{4}$-Ba1-$O4^{1}$	119.28(8)	$O1^{19}$-Ca1-$O1^{18}$	119.16(2)
$O1^{4}$-Ba1-$O4^{2}$	125.38(8)	$O2^{21}$-Ca1-$O1^{18}$	63.26(11)
O1-Ba1-O4	54.62(8)	$O2^{21}$-Ca1-$O1^{19}$	67.23(11)
$O1^{1}$-Ba1-O4	125.38(8)	$O2^{22}$-Ca1-$O1^{18}$	130.00(11)
O1-Ba1-$O4^{3}$	60.72(8)	$O2^{10}$-Ca1-$O1^{18}$	67.23(11)
$O1^{1}$-Ba1-$O4^{3}$	119.28(8)	$O2^{10}$-Ca1-$O1^{20}$	63.26(11)
$O1^{5}$-Ba1-$O4^{5}$	54.62(8)	$O2^{21}$-Ca1-$O1^{20}$	130.00(11)
$O1^{5}$-Ba1-$O4^{2}$	119.28(8)	$O2^{10}$-Ca1-$O1^{19}$	130.00(11)
$O1^{1}$-Ba1-$O4^{1}$	54.62(8)	$O2^{22}$-Ca1-$O1^{20}$	67.23(11)
$O1^{2}$-Ba1-$O4^{3}$	121.50(9)	$O2^{22}$-Ca1-$O1^{19}$	63.26(11)
$O1^{2}$-Ba1-$O4^{1}$	60.72(8)	$O2^{22}$-Ca1-$O2^{10}$	76.07(11)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O1-Ba1-O4[1]	125.38(8)	O2[21]-Ca1-O2[10]	76.07(11)
O1[5]-Ba1-O4[1]	121.50(9)	O2[21]-Ca1-O2[22]	76.07(11)
O1[5]-Ba1-O4[3]	125.38(8)	O3[7]-Ca1-O1[18]	147.24(11)
O1[3]-Ba1-O4	121.50(9)	O3-Ca1-O1[18]	66.94(9)
O1[2]-Ba1-O4[2]	54.62(8)	O3-Ca1-O1[20]	73.74(9)
O1[3]-Ba1-O4[4]	119.28(8)	O3[12]-Ca1-O1[20]	147.24(11)
O1[1]-Ba1-O4[5]	60.72(8)	O3[12]-Ca1-O1[19]	66.94(9)
O1[3]-Ba1-O4[2]	60.72(8)	O3-Ca1-O1[19]	147.24(11)
O4[4]-Ba1-O4[5]	101.98(7)	O3[7]-Ca1-O1[20]	66.94(9)
O4[4]-Ba1-O4	101.98(7)	O3[7]-Ca1-O1[19]	73.74(9)
O4[3]-Ba1-O4[5]	180.00(13)	O3[12]-Ca1-O1[18]	73.74(9)
O4[4]-Ba1-O4[1]	78.02(7)	O3[7]-Ca1-O2[21]	140.70(11)
O4[2]-Ba1-O4	78.02(7)	O3[12]-Ca1-O2[22]	130.12(11)
O4[2]-Ba1-O4[3]	101.98(7)	O3-Ca1-O2[22]	140.70(11)
O4[2]-Ba1-O4[5]	78.02(7)	O3[12]-Ca1-O2[10]	140.70(11)
O4[4]-Ba1-O4[3]	78.02(7)	O3[7]-Ca1-O2[22]	82.70(10)
O4[2]-Ba1-O4[1]	101.98(7)	O3-Ca1-O2[21]	130.12(11)
O4-Ba1-O4[1]	180	O3[12]-Ca1-O2[21]	82.70(10)
O4-Ba1-O4[5]	78.02(7)	O3-Ca1-O2[10]	82.70(10)
O4[3]-Ba1-O4[1]	78.02(7)	O3[7]-Ca1-O2[10]	130.12(11)
O4[5]-Ba1-O4[1]	101.98(7)	O3[12]-Ca1-O3[7]	86.40(12)
O4-Ba1-O4[3]	101.98(7)	O3-Ca1-O3[7]	86.40(12)
O4[4]-Ba1-O4[2]	180.00(13)	O3-Ca1-O3[12]	86.40(12)

Symmetry transformations used to generate equivalent atoms:

[1]-X,-Y,-Z; [2]-Y,+X-Y,+Z; [3]-Y+X,+X,-Z; [4]+Y,-X+Y,-Z; [5]+Y-X,-X,+Z; [6]-Y+X,+X,1/2+Z; [7]1+Y-X,1-X,+Z; [8]1+Y-X,1-X,1/2-Z; [9]1-X,1-Y,-1/2+Z; [10]1-X,1-Y,1-Z; [11]+X,+Y,1/2-Z; [12]1-Y,+X-Y,+Z; [13]1-X,-Y,-1/2+Z; [14]1-Y,+X-Y,1/2-Z; [15]+Y,-X+Y,-1/2+Z; [16]1-X,-Y,1/2+Z; [17]1+Y,1-X+Y,1/2+Z; [18]+Y,-X+Y,1/2+Z; [19]1-Y+X,+X,1/2+Z; [20]1-X,1-Y,1/2+Z; [21]+Y,-X+Y,1-Z; [22]1-Y+X,+X,1-Z; [23]-X,-Y,1/2+Z