Supporting Information

Multianvil High-Pressure/High-Temperature Synthesis and Characterization of magnetoelectric HP-Co_3TeO_6

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X-ray powder diffraction and Rietveld refinement:

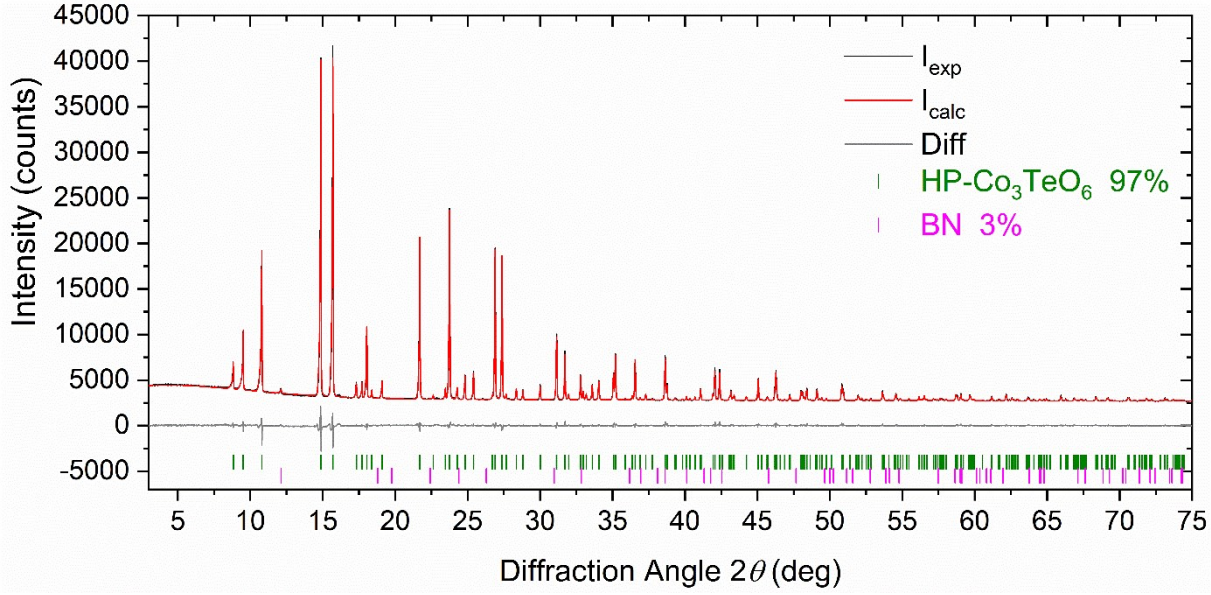

Figure SI1. XRD pattern (Mo-$K_{\alpha 1}$ radiation) and Rietveld refinement of HP-Co_3TeO_6 (R_{exp} = 3.41, R_{wp} = 6.40, R_p = 4.83, and *GOF* = 1.88). The curve of the experimental and calculated diffraction data are plotted with an offset of 2500 counts to better separate them from the difference curve.

Additional crystal structure data:

Table SI1: Anisotropic displacement parameters (Å^2) for HP-Co_3TeO_6, (*R*3, standard deviations in parentheses).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te	0.00439(9)	0.00439(9)	0.0049(2)	0	0	0.00220(5)
Co1	0.0069(2)	0.0069(2)	0.0070(4)	0	0	0.0034 (1)
Co2	0.0064(2)	0.0064(2)	0.0099(12)	0	0	0.00322(8)
Co3	0.0062(2)	0.0062(2)	0.0103(5)	0	0	0.0031 (1)
O1	0.006(1)	0.008(2)	0.008(1)	-0.0007(8)	0.0002(8)	0.0032(9)
O2	0.008(2)	0.007 (2)	0.0071(9)	-0.0013(8)	-0.0022(8)	0.003 (1)

Table SI2. Selected interatomic distances (pm) of HP-Co_3TeO_6 and Ni_3TeO_6 [1] as well as bond length discrepancies (pm) within the TeO_6-, CoO_6- and NiO_6-octahedra (standard deviations in parentheses).

Bond lengths of HP-Co_3TeO_6				**Bond lengths of Ni_3TeO_6 [1]**				**Bond length discrepancy per octhahedra for HP-Co_3TeO_6/ Ni_3TeO_6**
Te:	O1	195.7(4)	3×	Te:	O1	192.3 (5)	3×	4.3/ 3.3
	O2	191.4(3)	3×		O2	195.6 (5)	3×	
Co1:	O1	223.0(3)	3×	Ni1:	O1	203.2 (6)	3×	18.1/ 11.6
	O2	204.9(4)	3×		O2	214.8 (5)	3×	
Co2:	O1	203.7(4)	3×	Ni2:	O1	204.0 (6)	3×	18.7/ 9.9
	O2	222.4(3)	3×		O2	213.9 (7)	3×	
Co3:	O1	203.2(4)	3×	Ni3:	O1	200.8 (6)	3×	15.7/ 10.2
	O2	218.9(3)	3×		O2	211.0 (5)	3×	

Table SI3. Selected interatomic angles (°) of HP-Co_3TeO_6 and Ni_3TeO_6 [1]. Interatomic angle discrepancies (°), calculated on the deviation from the ideal value, are given in column 3 (standard deviations in parentheses).

Interatomic angles of HP-Co_3TeO_6			**Interatomic angles of Ni_3TeO_6 [1]**			**Interatomic angle discrepancy for HP-Co_3TeO_6/ Ni_3TeO_6**
O1-Te-O1	84.2(2)	3×	O1-Te-O1	83.6(2)	3×	5.8/ 6.4
O1-Te-O2	87.1(2)	3×	O1-Te-O2	86.8(3)	3×	2.9/ 3.2
O1-Te-O2	91.4(2)	3×	O1-Te-O2	91.8(3)	3×	1.4/ 1.8
O1-Te-O2	170.6(2)	3×	O1-Te-O2	169.8(3)	3×	9.4/ 10.2
O2-Te-O2	96.7(2)	3×	O2-Te-O2	97.0(3)	3×	3.3/ 3.0
O1-Co1-O1	72.1(2)	3×	O1-Ni1-O1	74.8(2)	3×	17.9/ 15.2
O1-Co1-O2	86.9(2)	3×	O1-Ni1-O2	87.8(3)	3×	3.1/ 2.2
O1-Co1-O2	88.3(2)	3×	O1-Ni1-O2	89.5(3)	3×	1.7/ 0.5
O1-Co1-O2	154.6(2)	3×	O1-Ni1-O2	159.0(3)	3×	25.4/ 21.0
O2-Co1-O2	106.9(2)	3×	O2-Ni1-O2	104.0(3)	3×	16.9/ 14.9
O1-Co2-O1	101.4(2)	3×	O1-Ni2-O1	99.5(3)	3×	11.4/ 9.5
O1-Co2-O2	87.3(2)	3×	O1-Ni2-O2	87.9(3)	3×	2.7/ 2.1
O1-Co2-O2	88.9(2)	3×	O1-Ni2-O2	89.9(3)	3×	2.1/ 1.1

O1-Co2-O2	164.7(2)	3×	O1-Ni2-O2	166.9(3)	3×	15.3/ 13.1
O2-Co2-O2	80.2(2)	3×	O2-Ni2-O2	81.2(3)	3×	9.8/ 8.8
O1-Co3-O1	106.4(2)	3×	O1-Ni3-O1	103.5(3)	3×	16.4/ 13.5
O1-Co3-O2	78.3(2)	3×	O1-Ni3-O2	80.7(3)	3×	12.7/ 9.3
O1-Co3-O2	90.8(2)	3×	O1-Ni3-O2	91.5(3)	3×	0.8/ 1.5
O1-Co3-O2	159.6(2)	3×	O1-Ni3-O2	162.8(3)	3×	20.4/ 17.2
O2-Co3-O2	81.8(2)	3×	O2-Ni3-O2	82.6(3)	3×	8.2/ 7.4

Band gap determination

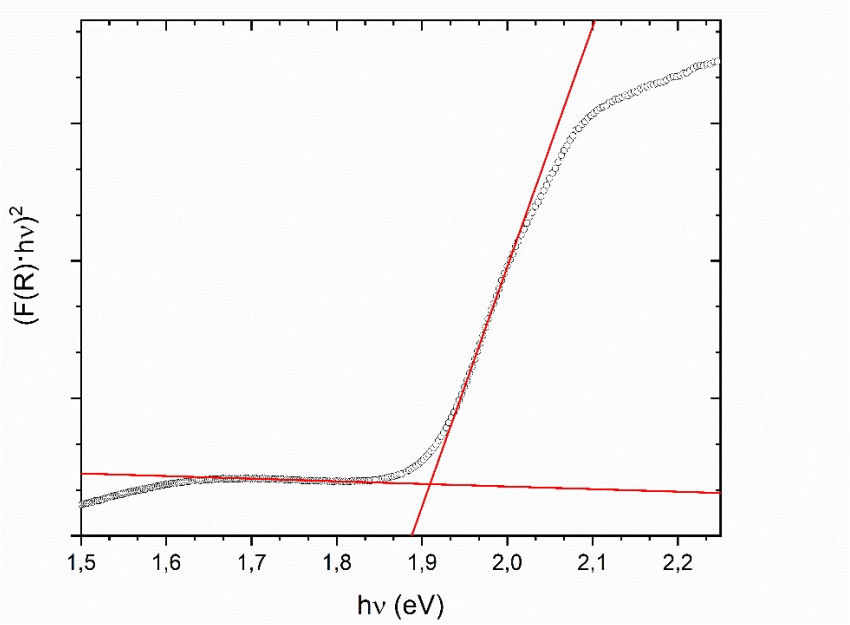

Figure SI2. Tauc plot for the band gap determination with n = 2.

Low field magnetic measurements

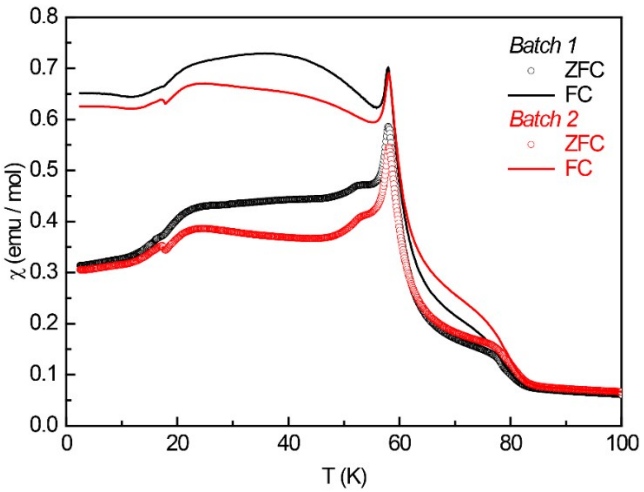

Figure SI3. *Zero-field-cooled / field-cooled* data (ZFC/FC) of HP-Co_3TeO_6 measured at 100 Oe.

Specific heat

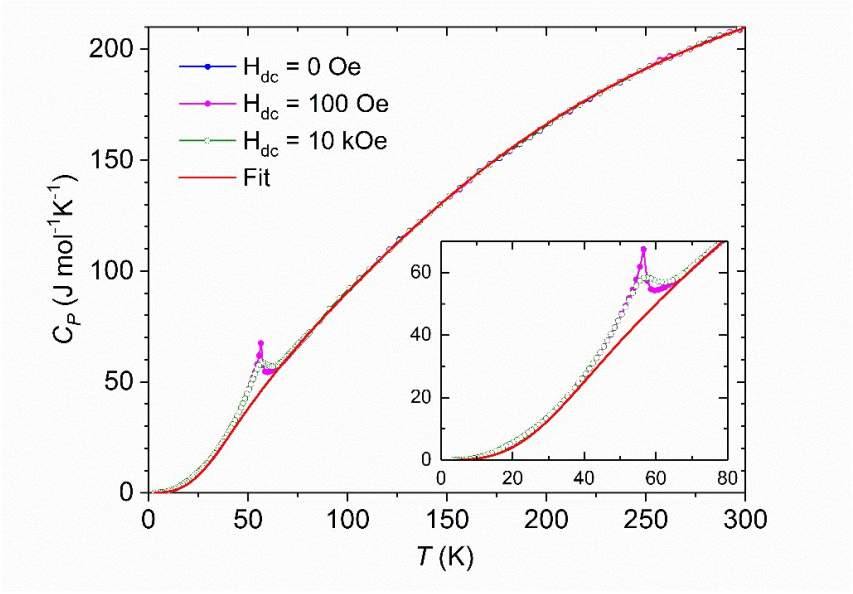

Figure SI4. Temperature dependence of the specific heat of HP-Co_3TeO_6 at H_{dc} = 0 Oe, 100 Oe and 10 kOe plus Einstein-Debye fit (red line) of the phonon contribution. Values at 0 Oe and 100 Oe are very similar and therefore not distinguishable.

Magnetoelectric properties

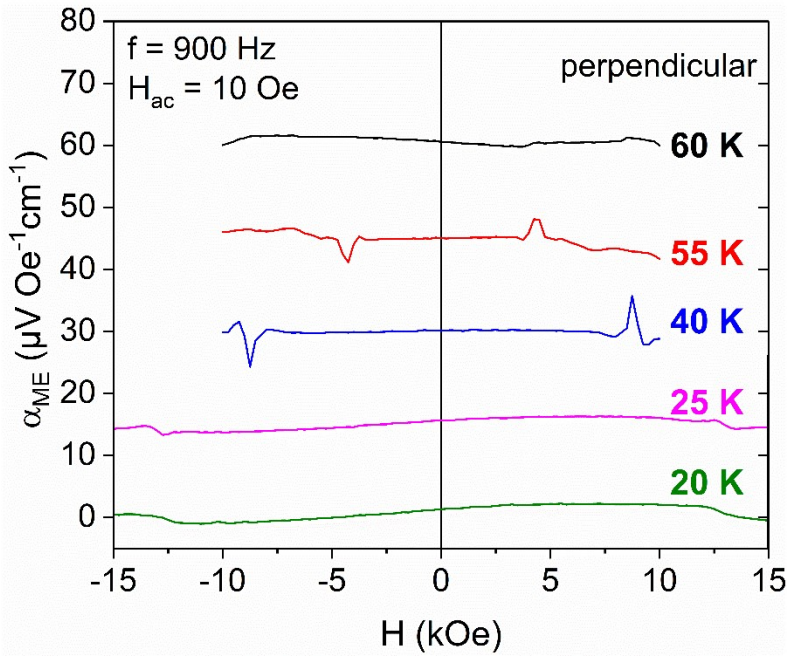

Figure SI5. Field dependence of the perpendicular magnetoelectric coefficient measured at different temperatures. Values recorded above 20 K are depicted with an offset.

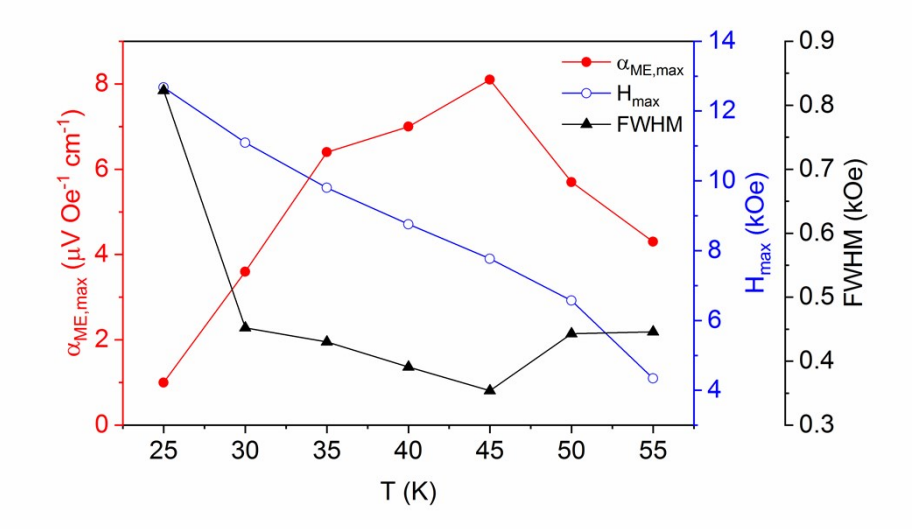

Figure SI6. Amplitude, field position and full width at half maximum of the α_{ME} peak measured in perpendicular geometry.

1. R. Becker and H. Berger, *Acta Crystallogr. E*, 2006, **62**, i222-i223.