Electronic Supplementary Information

Synthesis and characterisation of the vibrational and electrical properties of antiferromagnetic 6L-Ba_2CoTeO_6 ceramics

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Rietveld refinements were done using FULLPROF (Rodríguez-Carvajal, J. (1993). Phys. B: Condens. Matter, 192, 55–69.) The 6L-trigonal perovskite structure, space group P-3m (S. A. Ivanov, P. Nordblad, R. Mathieu, R. Tellgren and C. Ritter, Dalton Transactions, 2010, 39, 5490-5499) was used as a starting model for Rietveld refinements.

Colour was measured using a X-rite RM 200 QC colorimeter and reported in CIE LAB coordinates.

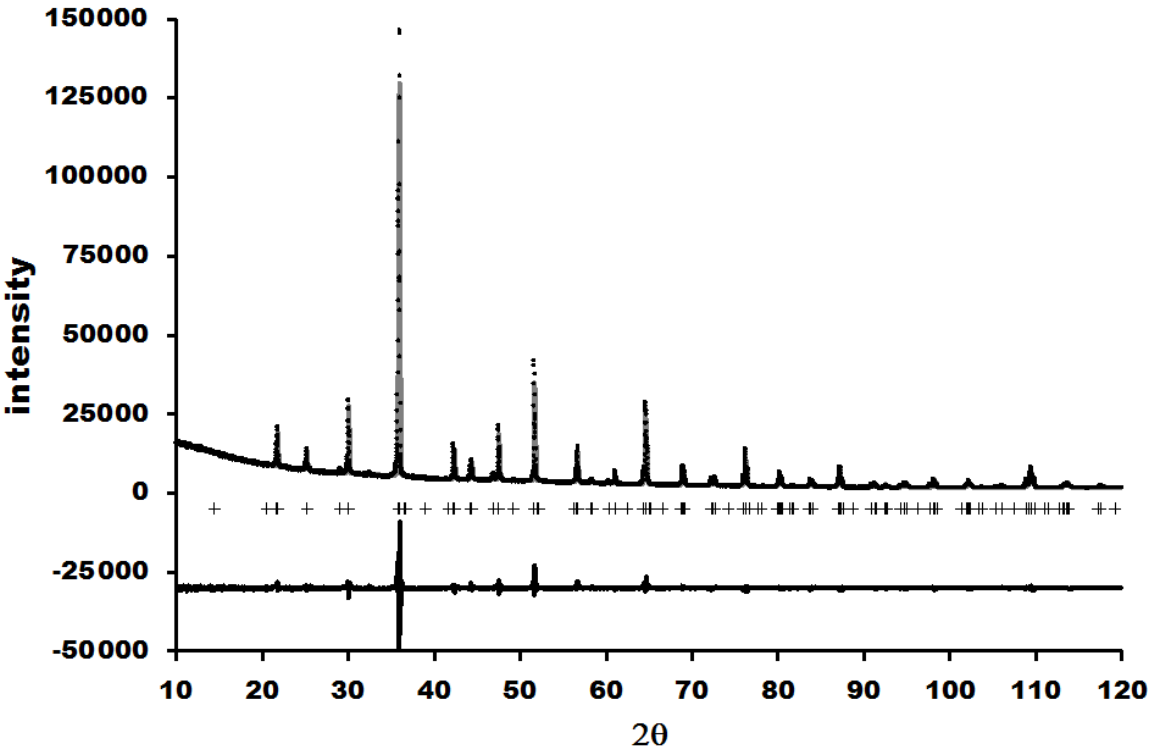


Figure S1. Room-temperature XRD data for Ba_2CoTeO_6 powder prepared at 1000 ℃.

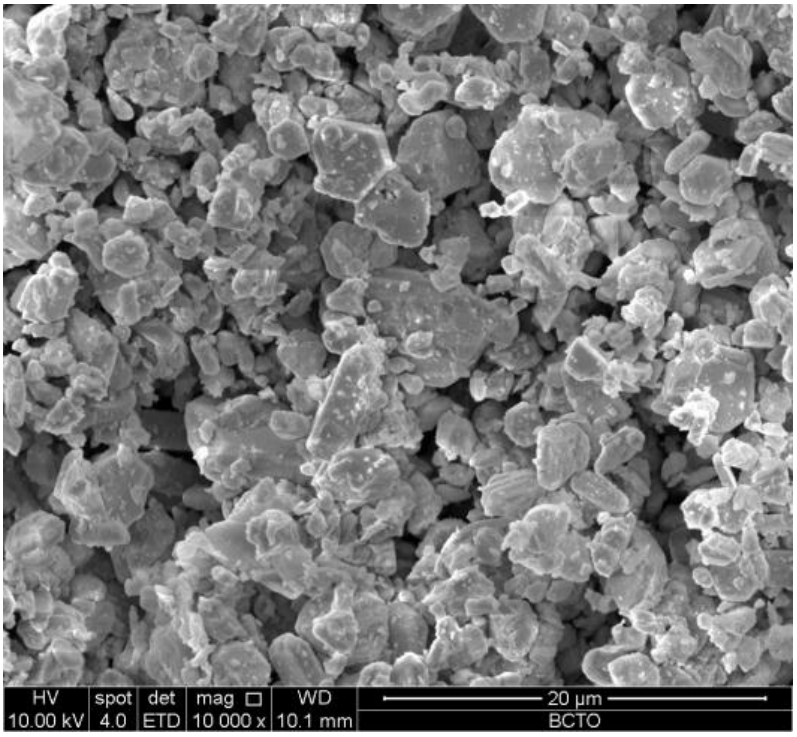
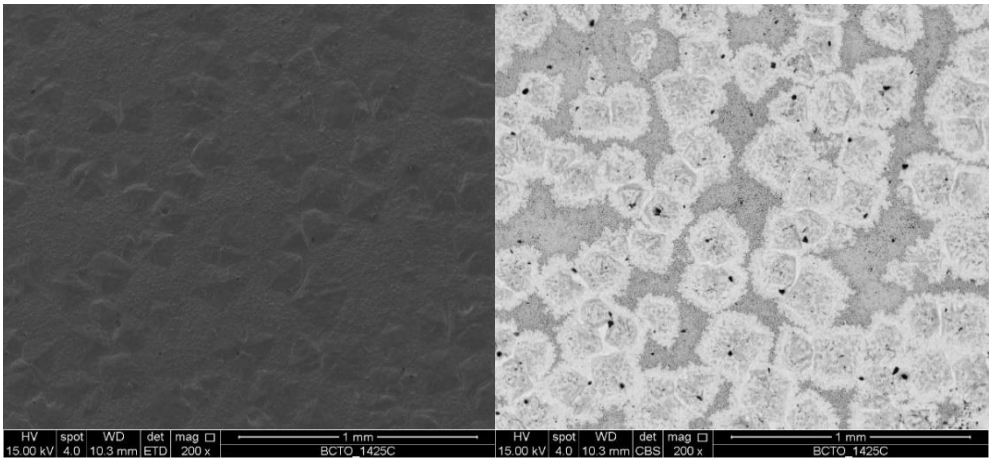
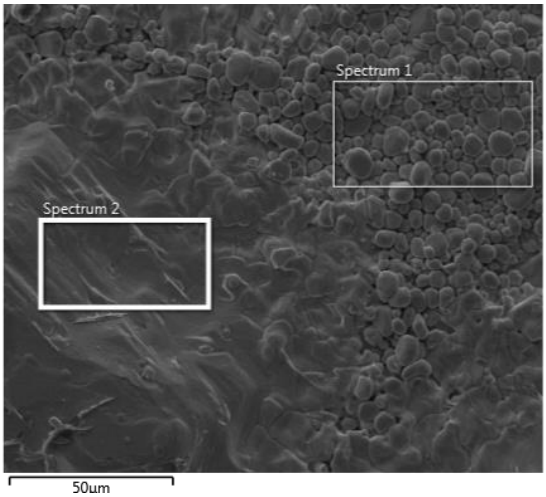
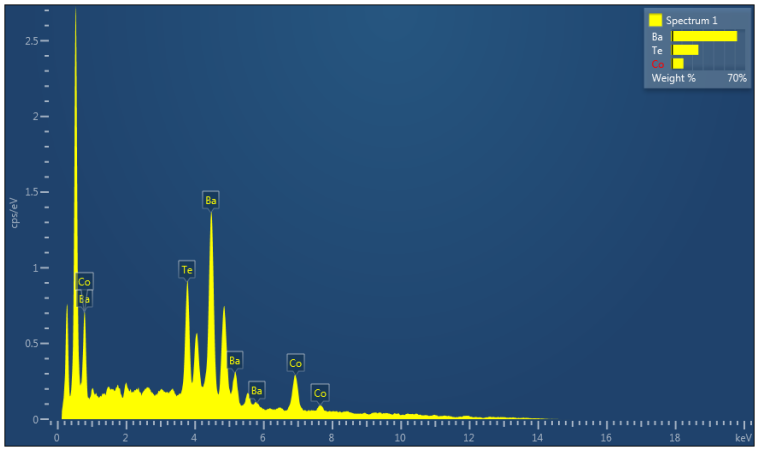


Figure S2. SEM micrograph showing the characteristics of the initial Ba_2CoTeO_6 powder.

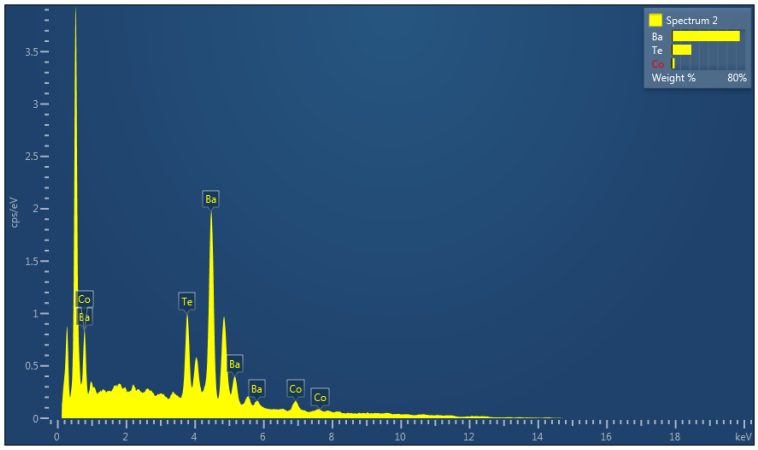


(a) SEI (b) BEI





Element	Line Type	Atomic %	Standard Label
Co	K	23.35	Co
Te	L	23.65	HgTe
Ba	L	53.00	BaF2
Total:		100.00	



Element	Line Type	Atomic %	Standard Label
Co	K	8.49	Co
Te	L	22.17	HgTe
Ba	L	69.34	BaF2
Total:		100.00	

(c) EDAX spectra from region 1 and 2.

Figure S3. (a)SEI, (b) BEI and (c) EDAX spectra from the two different regions of the as-fired surface of BCTO ceramics fired at 1425 ℃.

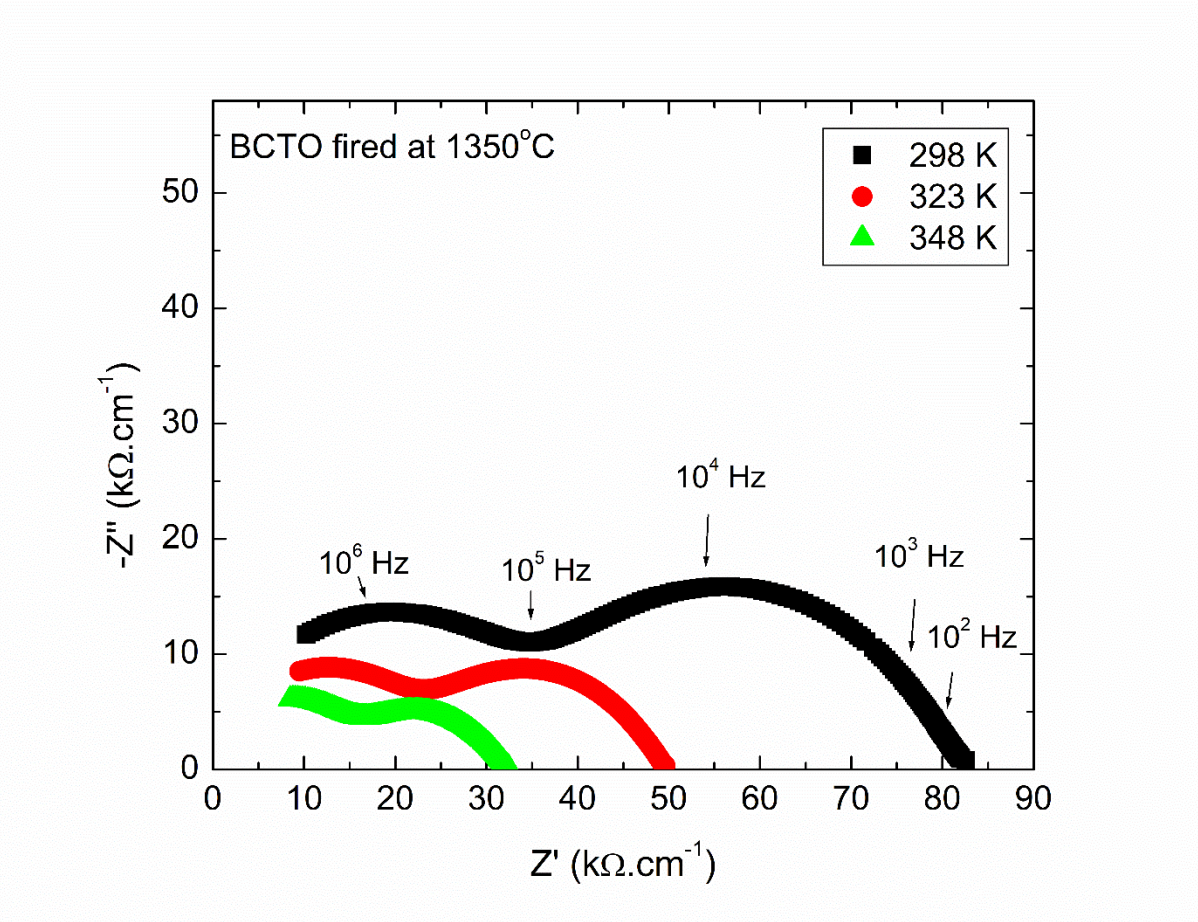


Figure S4. Z plot for BCTO ceramics fired at 1350 ℃.*

Table S1 – Firing schedule for powder synthesis and colour variation in the CIELAB colour space.

Firing Schedule	Mixed raw materials	500°C (12 h)	700°C (12 h)	900°C (12 h)	1000°C 2×(24 h)
CIE LAB coordinates					
L*	67.4	63.1	62.1	52.7	50.6
a*	-2.2	-1.3	-1.6	0.4	11.6
b*	-1.3	-0.3	-0.1	-3.4	-26.5
C*	2.5	1.3	1.6	3.5	29
h*	211.5	193.2	181.9	276.9	293.6

Table S2 – Refined Structural Parameters for BCTO. (Space group $P\bar{3}m1$)

Lattice parameters (Å)			Volume	*R* factors (%)		
a	b	c	(Å^3)	R_{wp}	R_p	χ^2
5.79870(3)	5.79870(3)	14.26599(9)	415.426(4)	26.5	19.1	21.87
	x	y	z	Uiso		Occ.
Ba(1)	0.00000	0.00000	0.2480(6)	0.0239(17)		1.00000
Ba(2)	0.33330	0.66670	0.0895(4)	0.024(2)		1.00000
Ba(3)	0.33330	0.66670	0.4005(4)	0.035(2)		1.00000
Co(1)	0.00000	0.00000	0.00000	0.030(8)		1.00000
Co(2)	0.33330	0.66670	0.6403(11)	0.036(5)		1.00000
Te(1)	0.00000	0.00000	0.50000	0.015(3)		1.00000
Te(2)	0.33330	0.66670	0.8381(4)	0.0155(17)		1.00000
O(1)	0.5021(18)	0.4979(18)	0.239(2)	0.011(6)		1.00000
O(2)	0.818(2)	0.182(2)	0.0754(17)	0.018(9)		1.00000
O(3)	0.848(3)	0.152(3)	0.4168(13)	0.009(8)		1.00000

Table S3 – Dependence of the relative density (%) in function of the firing temperature.

Firing temperature (°C)	Relative density (%)
1300	64
1350	87
1400	90
1425	80

Table S4 – Normal vibrational modes of BCTO at the Brillouin zone center (Γ-point), within the $\boldsymbol{P\bar{3}m1}$*, (#164 or* $\boldsymbol{D_{3d}^{3}}$*) hexagonal space group, with* Z_u *(=*Z_p*) = 3 (three motifs per unit or primitive cells).*

Ion	Wyckoff site[1]	Site symmetry	Irreducible representations
$Ba^{2+}(1)$	2c	C_{3v}	$A_{1g} \oplus A_{2u} \oplus E_g \oplus E_u$
$Ba^{2+}(2)$	2d	C_{3v}	$A_{1g} \oplus A_{2u} \oplus E_g \oplus E_u$
$Ba^{2+}(3)$	2d	C_{3v}	$A_{1g} \oplus A_{2u} \oplus E_g \oplus E_u$
$Co^{2+}(1)$	1a	D_{3d}	$A_{2u} \oplus E_u$
$Co^{2+}(2)$	2d	C_{3v}	$A_{1g} \oplus A_{2u} \oplus E_g \oplus E_u$
$Te^{6+}(1)$	1b	D_{3d}	$A_{2u} \oplus E_u$
$Te^{6+}(2)$	2d	C_{3v}	$A_{1g} \oplus A_{2u} \oplus E_g \oplus E_u$
$O^{2-}(1)$	6i	C_s	$2A_{1g} \oplus A_{1u} \oplus A_{2g} \oplus 2A_{2u} \oplus 3E_g \oplus 3E_u$
$O^{2-}(2)$	6i	C_s	$2A_{1g} \oplus A_{1u} \oplus A_{2g} \oplus 2A_{2u} \oplus 3E_g \oplus 3E_u$
$O^{2-}(3)$	6i	C_s	$2A_{1g} \oplus A_{1u} \oplus A_{2g} \oplus 2A_{2u} \oplus 3E_g \oplus 3E_u$
			$\boldsymbol{\Gamma_{acoustic} = A_{2u} \oplus E_u}$
			$\boldsymbol{\Gamma_{IR} = 12A_{2u} \oplus 15E_u}$
			$\boldsymbol{\Gamma_{Raman} = 11A_{1g} \oplus 14E_g}$
			(Silent: $3A_{1u} \oplus 3A_{2g}$)