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A Facilitated Method to Grow Crystals of Cobalt Tellurite Multiferroic Material Co_3TeO_6

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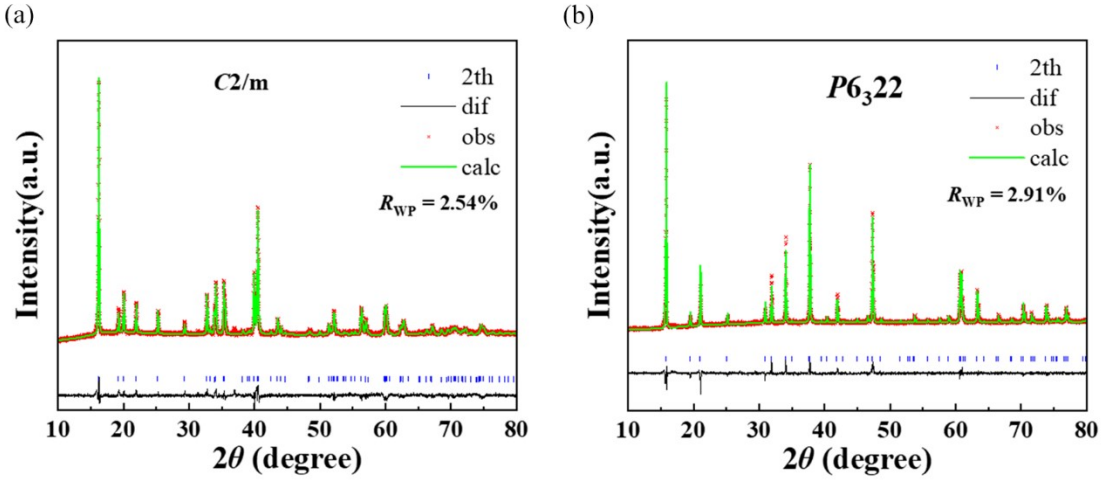

Fig. S1 The Rietveld refinement of polymorphs $Na_2Co_2TeO_6$, yielding the unit-cell parameters (a) a = 5.3521(1) Å, b = 9.2380(1) Å, c = 5.7898(1) Å and β= 108.899(1)° for monoclinic polymorph and (b) $a = b$ = 5.2732(1) Å, c = 11.2421(1) Å and γ = 120° for hexagonal one, respectively.

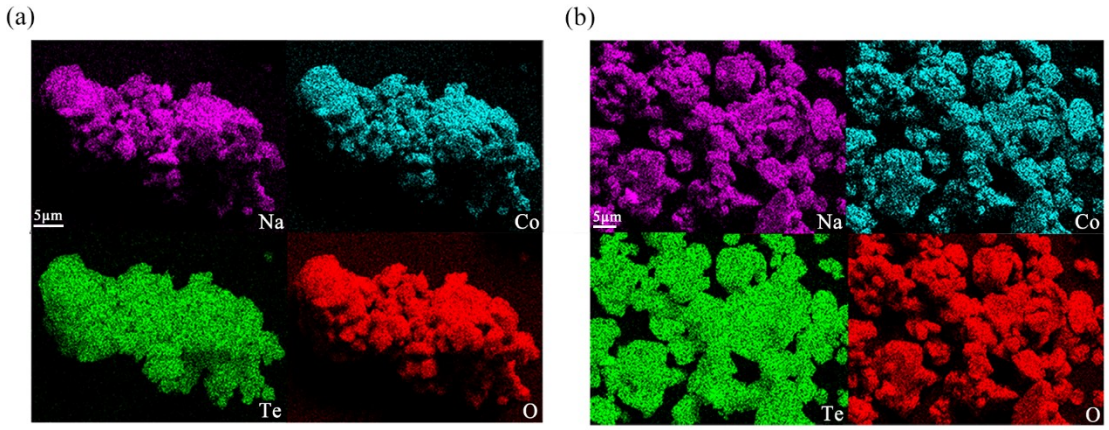

Fig. S2 The EDS of (a) monoclinic polymorph and (b) hexagonal polymorph of $Na_2Co_2TeO_6$, respectively.

Fig. S3 The EDS results of Co_3TeO_6 crystals using (a) monoclinic $Na_2Co_2TeO_6$ as precursor, (b) the X-ray diffraction patterns of Co_3TeO_6 crystals and (c) EDS result using single crystals. Zone 1, zone 2 and zone 3 in Fig S3c represent the phases of Co_3TeO_6, Na_2MoO_4 and Na_2TeO_4, respectively.

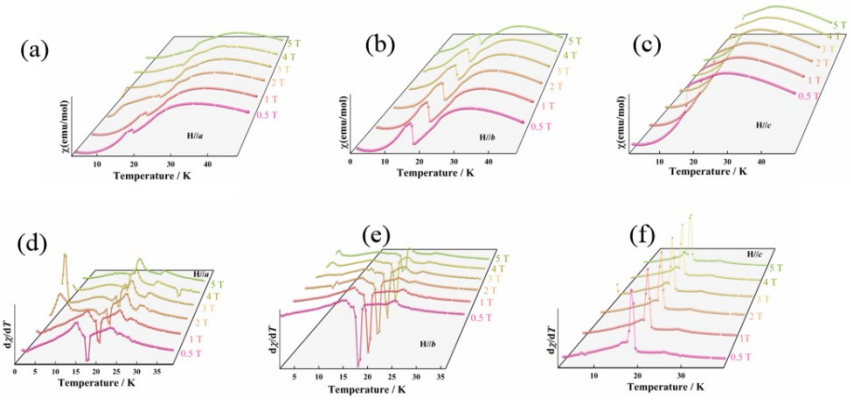

Fig. S4 The magnetic susceptibilities and its differential under various magnetic fields from 0.5 to 5 T along *a* (a,d), *b* (b,e) and *c* (c,f) axis.

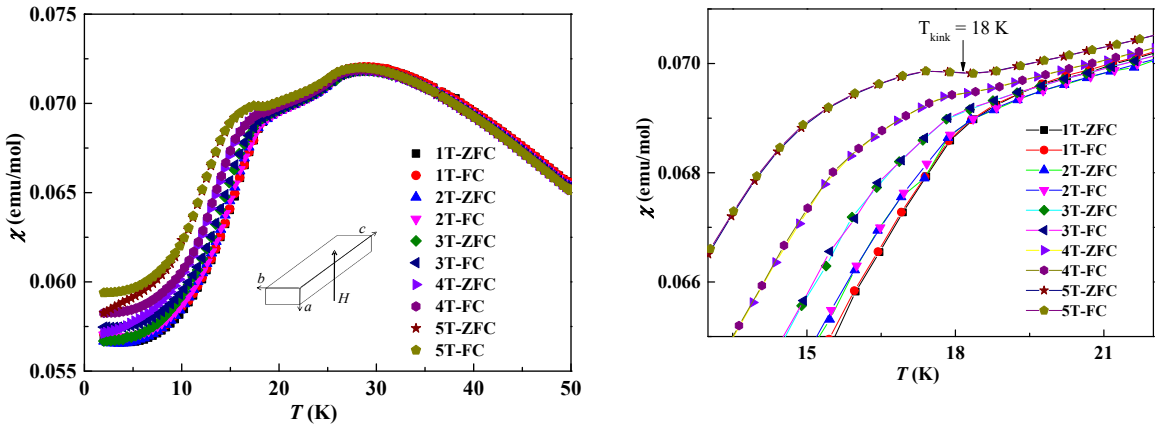

Fig. S5 The magnetic susceptibilities with external field from 1 T to 5 T parallel to Archimedean T11 lattice.

Table S1 The refined crystallographic parameters of polymorphs $Na_2Co_2TeO_6$.

Materials	$Na_2Co_2TeO_6$ Monoclinic	$Na_2Co_2TeO_6$ Hexagonal	
Space group	*C*2/m	$P6_322$	
a (Å),	5.3521(1),	5.2732(1),	
b (Å),	9.2380(1),	5.2732(1),	
c (Å)	5.7898(1)	11.2421(1)	
α , β , γ (°)	90, 108.899(1), 90	90, 90, 120	
Na1-4*h*, (*x, y, z*)	(0.5, 0.3243(10), 0.5)	Na1-12*i*, (*x, y, z*)	(0.2465, 0.65, -0.026)
		Na2-2*a*, (*x, y, z*)	(0, 0, 0)
Na2-2*d*, (*x, y, z*)	(0, 0.5, 0.5)	Na3-12*i*, (*x, y, z*)	(0.7181(29), 0.0677(29), 0.0060(24))
Co1-4*g*, (*x, y, z*)	(0, 0.6657(3), 0)	Co1-2*b*, (*x, y, z*)	(0, 0, 0.25)
		Co2-2*d*, (*x, y, z*)	(2/3, 1/3, 0.25)
Te1-2*a*, (*x, y, z*)	(0, 0, 0)	Te1-2*c*, (*x, y, z*)	(1/3, 2/3, 0.25)
O1-8*j*, (*x, y, z*)	(0.2806(8), 0.3456(9), 0.8030(3))	O1-12*i*, (*x, y, z*)	(0.6432, -0.0252,0.3452)
O2-4i, (x, y, z)	(0.2647, 0.5, 0.1923)		
χ^2, R_{wp} (%), R_p (%)	1.63, 2.54, 1.85	1.78, 2.91, 1.88	

Table S2 The Structural refinement parameters of single-crystal Co_3TeO_6.

Empirical formula	Co_3TeO_6
Formula weight / g/mol	400.39
Temperature / K	100.00(10)
Crystal system	Monoclinic
Space group	*C*2/c
a / Å	14.7610(11)
b / Å	8.8319(6)
c / Å	10.3387(8)
β /°	95.102(7)
Volume / Å^3	1342.49(17)
ρ_{calc} / g/cm^3	5.943
μ / mm^{-1}	17.328
F(000)	2172.0
Crystal size / mm^3	0.96 × 0.73 × 0.58
Radiation Mo$K\alpha$	Mo $K\alpha$ (λ = 0.71073 Å)
2θ range for data collection / °	5.380 to 61.642
Index ranges	-19 ≤ h ≤ 21, -11 ≤ k ≤ 11,-14 ≤ l ≤ 14
Reflections collected	4934
Independent reflections	1787
Goodness-of-fit on F^2	1.073
Final *R* indexes [I >= 2σ (I)]	R_1 = 0.0600,
Final *R* indexes [all data]	R_1 = 0.0635,

$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$, $wR_2 = \{\sum w[(F_o)^2 - (F_c)^2]^2/\sum w[(F_o)^2]^2\}^{1/2}$

Table S3 Summary of exemplary crystal growth of tellurides.

Compound	Raw materials	Method	Magnetism	Space group	Reference
$CoTe_6O_{13}$	$BaCO_3$, TeO_2, $CoCl_2.6H_2O$	Hydrothermal synthesis	T_N = 21 K, AFM	$R\bar{3}$	1
$MnTe_6O_{13}$	$MnCl_2.4H_2O$, TeO_2	Hydrothermal synthesis	T_N = 13 K, AFM	$R\bar{3}$	1
$Na_2Co_2Te_6$	Na_2O, Co_3O_4, TeO_2	Flux Method	T_N = 9.6 K, AFM	$P6_322$	2
$CoTeMoO_6$	$CoTeMoO_6$, TeO_2, MoO_3	Flux Method	T_N =23.44K, AFM	$P2_12_12$	3
Cu_3TeO_6	CuO, TeO_2, $PbCl_2$	Flux Method	T_N = 60 K, AFM	$Ia\bar{3}$	4
Ni_3TeO_6	NiO, CuO, TeO_2, $NiCl_2$	Chemical vapor transport	T_N = 52 K, AFM	$R3$	5
$CoTeO_4$	$CoTeO_4$, H_6TeO_6, $Co(NO_3)_2(H_2O)_6$	Chemical vapor transport	T_N = 50 K, AFM	$P21/n$	6
Pb_2CoTeO_6	PbO, CoO, TeO_2	Flux Method	T_N = 16 K, AFM	$R\bar{3}$	7
$CaCo_4(TeO_3)_4Cl_2$	CaO, $CoCl_2$, CoO, TeO_2	Flux Method	T_N = 11.5 K, AFM	$C2/c$	8
Mn_3TeO_6	MnO, TeO_3, $PtCl_2$	Chemical vapor transport	T_N = 23 K, AFM	$R\bar{3}$	9
$Na_2Ni_2TeO_6$	$Na_2Ni_2TeO_6$, Na_2O, TeO_2	Flux method	T_N = 25 K, AFM	$P6_322$	10
Co_3TeO_6	Co_3TeO_6, $PbCl_2$	Flux method	T_N = 26 K, AFM	$C2/c$	11
Co_3TeO_6	Co_3TeO_6, $PtCl_2$ or HCl	Chemical vapor transport	T_N = 26 K, AFM	$C2/c$	12,13
Co_3TeO_6	$Na_2Co_2TeO_6$, MoO_3	Flux method	T_N = 26 K, AFM	$C2/c$	this work

Reference

1 J. T. S. Irvine, M. G. Johnston and W. T. A. Harrison, *Dalton Trans.*, 2003, **13**, 2641-2645.
2 G. Xiao, Z. Xia, W. Zhang, X. Yue, S. Huang, X. Zhang, F. Yang, Y. Song, M. Wei, H. Deng and D. Jiang, *Cryst. Growth Des.*, 2019, **19**, 2658–2662.
3 M. Mączka, K. Hermanowicz, A. Majchrowski, Ł. Kroenke, A. Pietraszko and M. Ptak, *J. Solid State Chem.*, 2014, **220**, 142–148.
4 K. Y. Choi, P. Lemmens, E. S. Choi and H. Berger, *J. Phys.: Condens. Matter.*, 2008, **20**, 505214.
5 I. Živković, K. Prša, O. Zaharko and H. Berger, *J. Phys.: Condens. Matter.*, 2010, **22**, 056002.
6 P P. Pramanik, F. Eder, M. Weil, S. A. Ivanov, P. Maltoni, R. Miletich, T. Edvinsson and R. Mathieu, *Phys. Rev. B.*, 2024, **110**, 054104.
7 C. Artner and M. Weil, *J. Solid State Chem.*, 2019, **276**, 75–86.
8 K. Stolze, T. Kong, F. O. Von Rohr and R. J. Cava, *J. Solid State Chem.*, 2018, **263**, 141–147.
9 S. A. Ivanov, P. Nordblad, R. Mathieu, R. Tellgren, C. Ritter, N. V. Golubko, E. D. Politova and M. Weil, *Mater. Res. Bull.*, 2011, **46**, 1870–1877.
10 R. Sankar, I. Panneer Muthuselvam, G. J. Shu, W. T. Chen, S. K. Karna, R. Jayavel and F. C. Chou, *CrystEngComm.*, 2014, **16**, 10791–10796.
11 C. B. Liu, C. C. Ma, T. Li, H. W. Wang, R. Chen, M. Y. Cui, J. B. Cheng, J. B. He, S. J. Jin, Y. S. Luo and J. F. Wang, *Phys. Rev. B.*, 2024, **109**, 214408.
12 M. Hudl, R. Mathieu, S. A. Ivanov, M. Weil, V. Carolus, Th. Lottermoser, M. Fiebig, Y. Tokunaga, Y. Taguchi, Y. Tokura and P. Nordblad, *Phys. Rev. B.*, 2011, **84**, 180404.
13 R. Becker, M. Johnsson and H. Berger, *Acta Crystallogr C Cryst Struct Commun.*, 2006, **62**, i67–i69.