Electronic Supplementary Material (ESI) for Dalton Transactions.

New β-$CdTeO_3$ Polymorph with related structure to α-$CdTeO_3$

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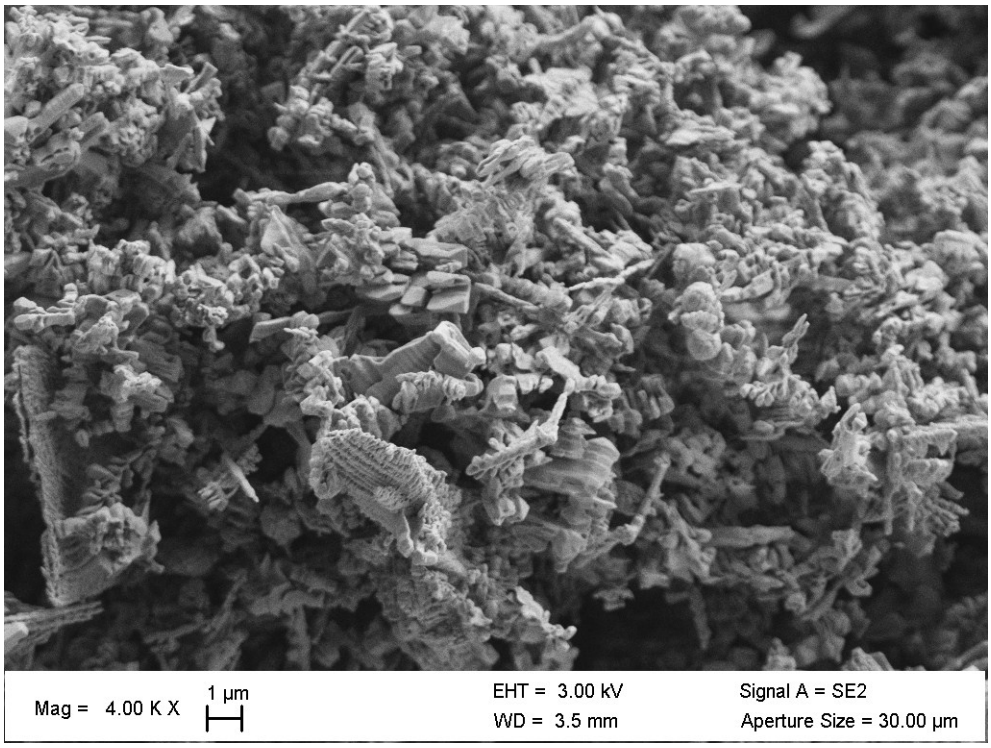

Figure s1. SEM image of a polycrystalline sample of β-$CdTeO_3$

Table s1. EDX quantitative analyses on β-$CdTeO_3$ cristallites

Element	**concentration (%-atomic)**			
	crystallite			
	1	2	3	average
Cd-L	48.9	51.9	50.8	50.5
Te-L	51.1	48.1	49.8	49.7

Table s2. Selected interatomic distances for α-$CdTeO_3$ calculated from the ICSD file number 60067.

Atom 1	Atom 2	Distance (Å)	Atom 1	Atom 2	Distance (Å)
Cd1	O5	2.1967(57)	Cd2	O6	2.2842(60)
	O6	2.2883(53)		O3	2.2931(64)
	O4	2.3068(60)		O4	2.2952(53)
	O1	2.3192(64)		O3	2.3178(61)
	O3	2.4327(61)		O1	2.3482(61)
	O5	2.4761(55)		O2	2.3645(60)
Te1	O2	1.8687(73)	Te2	O6	1.8687(56)
	O4	1.8822(52)		O1	1.8877(52)
	O5	1.8942(62)		O3	1.9160(62)
	O5	2.7628(63)		O2	2.5456(73)
				O1	2.7541(59)

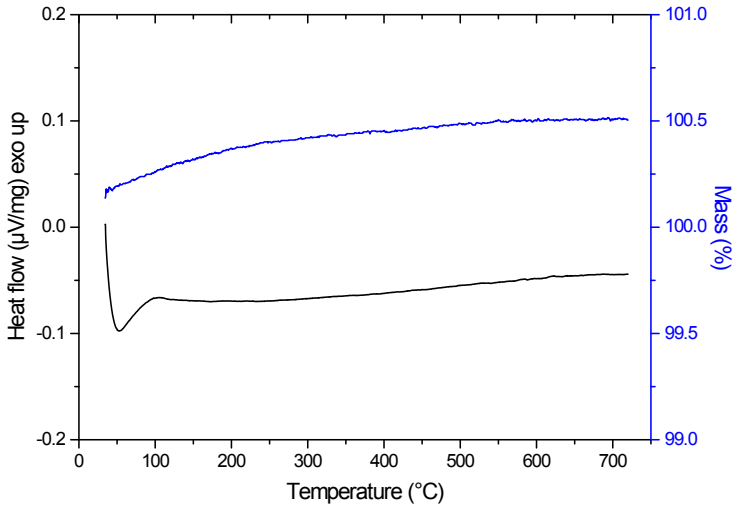

Figure s2. TG (blue) and DSC (brown) curves of β-$CdTeO_3$.

Table s3. Common subgroups of space groups *Pnma* (G_1; Z_1 = 16) and *P*21/*c* (G_2; Z_2 = 8) with maximum cell multiplication (for both branches) of 2.

	Common Subgroup H							Branch G_1 > H			Branch G_2 > H
N	**LEVEL**	**HM Symbol**	P_H	Z_H	**IT*A***	i_1	it_1	ik_1	i_2	it_2	ik_2
1	(1,1)	*P*2$_1$/*c*	2/m	16	14	2	2	1	2	1	2
2	(2,2)	*Pc*	m	16	7	4	4	1	4	2	2
3	(2,2)	*P*2$_1$	2	16	4	4	4	1	4	2	2
4	(2,2)	*P*-1	-1	16	2	4	4	1	4	2	2
5	(3,3)	*P*1	1	16	1	8	8	1	8	4	2

Table s4. Group-subgroup relations for transition path with *P*2$_1$/*c* (Z_H=16) as common subgroup

Unit cells (a,b,c,α,β,&gamma)	**Branch**	**(P,p)**	**Transformation matrix**
G_1 > H_1 G_1: 7.45877 14.52241 11.04631 90 90 90 H_1: 14.5224 11.0463 7.4588 90 90 90.00	*Pnma* > *P*2$_1$/*c* (index 2)	b,c,a	[0 0 1] [0] [1 0 0] [0] [0 1 0] [0]
G_2 > H_2 G_2: 7.790 11.253 7.418 90.000 113.5 90.000 H_2: 14.3386 11.2530 7.4180 90 85.18 90.00	*P*2$_1$/*c* > *P*2$_1$/*c* (index 2)	2a+c+1,b,c+1/2	[2 0 0] [1] [0 1 0] [0] [1 0 1] [1/2]

Table s5. Mappings of the atoms between β'-CdTeO3 (S1) and α'-CdTeO3 (S2)

WP		Atom in $\beta'CdTeO_3$	Coordinates (*x,y,z*) in S_1 : $\beta'CdTeO_3$	Atom in $\alpha'CdTeO_3$	Coordinates (x,y,z) in S_2 : $\alpha'CdTeO_3$	Related atom in α-$CdTeO_3$
4e	(x,y,z)	Cd1	(0.633060,0.980030,0.283140)	Cd1	(0.634950,0.008900,0.174650)	Cd1
4e	(x,y,z)	Cd1_2	(0.133060,0.019970,0.716860)	Cd1_2	(0.134950,0.008900,0.674650)	Cd1
4e	(x,y,z)	Cd2	(0.500670,0.232930,0.464830)	Cd2	(0.502100,0.267300,0.472900)	Cd2
4e	(x,y,z)	Cd2_2	(0.000670,0.767070,0.535170)	Cd2_2	(0.997900,0.767300,0.527100)	Cd2
4e	(x,y,z)	Te1	(0.250000,0.766370,0.690900)	Te1	(0.247200,0.755500,0.632200)	Te1
4e	(x,y,z)	Te2	(0.914980,0.500160,0.305940)	Te2	(0.916400,0.499200,0.322200)	Te2
4e	(x,y,z)	Te2_2	(0.414980,0.499840,0.694060)	Te2_2	(0.416400,0.499200,0.822200)	Te2
4e	(x,y,z)	Te3	(0.750000,0.770050,0.574700)	Te3	(0.747200,0.744500,0.632200)	Te1
4e	(x,y,z)	O1	(0.508000,0.368400,0.231300)	O1	(0.476800,0.409600,0.137700)	O1
4e	(x,y,z)	O1_2	(0.008000,0.631600,0.768700)	O1_2	(0.004100,0.630300,0.759100)	O3
4e	(x,y,z)	O2	(0.519200,0.092800,0.137800)	O2	(0.495900,0.130300,0.240900)	O3
4e	(x,y,z)	O2_2	(0.019200,0.907200,0.862200)	O2_2	(0.023200,0.909600,0.862300)	O1
4e	(x,y,z)	O3	(0.595000,0.574300,0.087600)	O3	(0.598000,0.424900,0.397800)	O6
4e	(x,y,z)	O3_2	(0.095000,0.425700,0.912400)	O3_2	(0.098000,0.424900,0.897800)	O6
4e	(x,y,z)	O4	(0.750000,0.097400,0.151600)	O4	(0.756400,0.127000,0.184500)	O5
4e	(x,y,z)	O5	(0.347400,0.674300,0.059300)	O5	(0.350200,0.680100,0.994800)	O2
4e	(x,y,z)	O5_2	(0.847400,0.325700,0.940700)	O5_2	(0.849800,0.331100,0.979800)	O4
4e	(x,y,z)	O6	(0.250000,0.343900,0.160000)	O6	(0.256400,0.373000,0.184500)	O5
4e	(x,y,z)	O7	(0.649200,0.833700,0.014100)	O7	(0.650200,0.831100,0.020200)	O4
4e	(x,y,z)	O7_2	(0.149200,0.166300,0.985900)	O7_2	(0.149800,0.180100,0.005200)	O2

Table s6. Atomic displacements for the transition path of β'$CdTeO_3$ (S1) in α'$CdTeO_3$ (S2)

Wyckoff Positions		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u| (Å)
4e	(x,y,z)	Cd1	0.0019	0.0289	-0.1085	0.8702
4e	(x,y,z)	Cd1_2	0.0019	-0.0111	-0.0422	0.3389
4e	(x,y,z)	Cd2	0.0014	0.0344	0.0081	0.385
4e	(x,y,z)	Cd2_2	-0.0028	0.0002	-0.0081	0.0724
4e	(x,y,z)	Te1	-0.0028	-0.0109	-0.0587	0.4558
4e	(x,y,z)	Te2	0.0014	-0.001	0.0163	0.1235
4e	(x,y,z)	Te2_2	0.0014	-0.0006	0.1281	0.956
4e	(x,y,z)	Te3	-0.0028	-0.0255	0.0575	0.515
4e	(x,y,z)	O1	-0.0312	0.0412	-0.0936	0.9486
4e	(x,y,z)	O1_2	-0.0039	-0.0013	-0.0096	0.0924
4e	(x,y,z)	O2	-0.0233	0.0375	0.1031	0.9367
4e	(x,y,z)	O2_2	0.004	0.0024	0.0001	0.0639
4e	(x,y,z)	O3	0.003	-0.1494	0.3102	2.8423
4e	(x,y,z)	O3_2	0.003	-0.0008	-0.0146	0.1176
4e	(x,y,z)	O4	0.0064	0.0296	0.0329	0.4192
4e	(x,y,z)	O5	0.0028	0.0058	-0.0645	0.487
4e	(x,y,z)	O5_2	0.0024	0.0054	0.0391	0.2997
4e	(x,y,z)	O6	0.0064	0.0291	0.0245	0.3813
4e	(x,y,z)	O7	0.001	-0.0026	0.0061	0.0557
4e	(x,y,z)	O7_2	0.0006	0.0138	0.0193	0.2098