Electronic Supplementary Information for:

Characterization and Optimization of the Growth Conditions of a Novel $Cs_2TeW_3O_{12}$ Piezoelectric Crystal

Peng Zhao,[a] Qian Wu,[a] Zeliang Gao,[a,b*] Xiangxin Tian,[a] Conggang Li,[a] Youxuan Sun,[a] Chengqian Zhang,[a] Shengqing Xia,[a] and Xutang Tao[a,b*]

[a] *State Key Laboratory of Crystal Materials, Shandong University, No.27 Shanda South Road, Jinan, 250100, China.*

[b] *Key Laboratory of Functional Crystal Materials and Device (Shandong University, Ministry of Education)，No.27 South Shanda Road, Jinan, 250100, China*

E-mail: txt@sdu.edu.cn; Fax: +86-531-88574135; Tel: +86-531-88364963; E-mail: gaozeliang@sdu.edu.cn

Figure S1. Ball-and-stick diagram of CTW in ac-plane. Note that CTW exhibits a two-dimensional layered structure along the c-direction. Every layer consists of wave-connected WO_6 octahedra, and TeO_3 polyhedra covering the same side of the W-O layer. The distance between these layers is 3.25 Å.

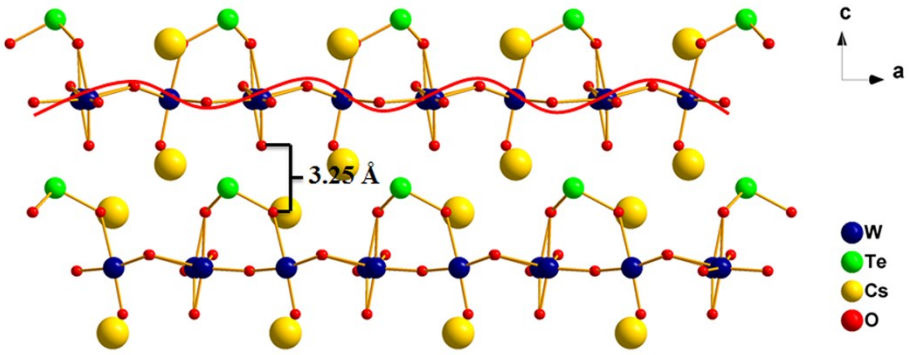

Figure S2. Directions of dipole moments of each WO_6 and TeO_3 polyhedra in the unit cell of CTW. Note that the light blue and green arrows indicate the directions of dipole moments for WO_6 and TeO_3 polyhedra, respectively. The red arrow indicates the direction of the net dipole moments of the unit cell.

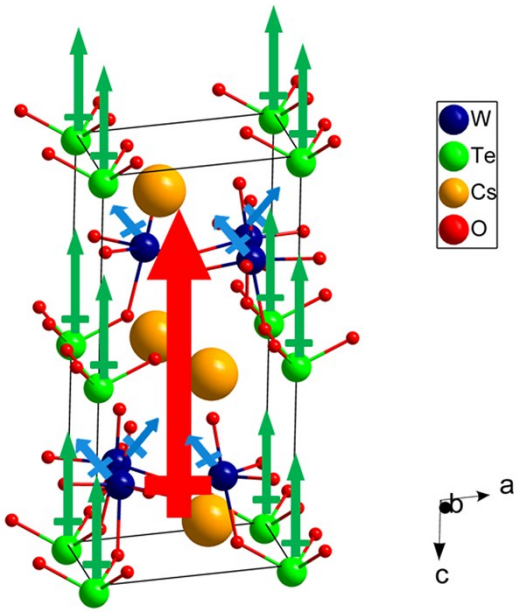

Figure S3. Atomic coordinates and dipole moment of CTW.

Atomic coordinates for $Cs_2TeW_3O_{12}$						
	x	y	z	x	y	z
W	0. 85407	1. 1928	0. 28018	6. 25854	8. 740719	3. 476333
01	1. 1267	1. 2493	0. 2706	8. 256345	9. 154745	3. 35747
01	0. 7507	0. 8774	0. 2706	5. 501055	6. 429499	3. 35747
02	0. 5483	1. 0883	0. 3184	4. 017888	7. 974954	3. 950548
02	0. 9117	1. 46	0. 3184	6. 680846	10. 69873	3. 950548
03	0. 8664	1. 1284	0. 4449	6. 348893	8. 268802	5. 520097
04	0. 8058	1. 1958	0. 1425	5. 904822	8. 762703	1. 768069
Te	0	0	0. 51674	0	0	6. 411452
03	−0. 1336	0. 1284	0. 4449	−0. 97901	0. 940902	5. 520097
03	−0. 1284	−0. 262	0. 4449	−0. 9409	−1. 91991	5. 520097
03	0. 262	0. 1336	0. 4449	1. 91991	0. 979007	5. 520097

WO_6 in CTW			Cart. Coord.			distance	unit vector				dipole moment for each		
Z	atom	charges	x	y	z	Å	x	y	z	unitized Vec	C_grav	C_charge	u_debye
74	W	6.09979	6.25854	8.74072	3.47633								
8	O1	-1.264	8.25635	9.15475	3.35747	2.044	-0.9775	-0.2026	0.05816	1	0.09756	0.12006	17.0313
8	O1	-0.709	5.50106	6.4295	3.35747	2.435	0.31107	0.94913	0.04881	1	0.09756	0.11368	14.4353
8	O2	-0.739	4.01789	7.97495	3.95055	2.415	0.92784	0.3171	-0.1964	1	0.09756	0.11403	14.6309
8	O2	-1.209	6.68085	10.6987	3.95055	2.058	-0.2052	-0.9512	-0.2304	1	0.09756	0.11943	16.662
8	O3	-0.594	6.34889	8.2688	5.5201	2.099	-0.043	0.22478	-0.9735	1	0.09756	0.11235	11.401
8	O4	-1.584	5.90482	8.7627	1.76807	1.745	0.20275	-0.0126	0.97915	1	0.09756	0.12369	16.9516
				Cell Volume		577			Dipole Moment			Magnitude	
				Z		2			x	y	z		
				Total Dipole Moment =			0.00606	esu*cm/A^3	0.9447	1.3899	0.4832	1.7486	debye

WO_6 in CTW			Cart. Coord.			distance	unit vector				dipole moment for each		
Z	atom	charges	x	y	z	Å	x	y	z	unitized Vec	C_grav	C_charge	u_debye
74	W	6.09979	0	0	0								
8	O1	-1.2644	-1.9978	-0.414	0.11886	2.044	-0.9775	-0.2026	0.05816	1	0.09756	0.12006	17.0313
8	O1	-0.7091	0.75749	2.31122	0.11886	2.435	0.31107	0.94913	0.04881	1	0.09756	0.11368	14.4353
8	O2	-0.7392	2.24065	0.76577	-0.4742	2.415	0.92784	0.3171	-0.1964	1	0.09756	0.11403	14.6309
8	O2	-1.2092	-0.4223	-1.958	-0.4742	2.058	-0.2052	-0.9512	-0.2304	1	0.09756	0.11943	16.662
8	O3	-0.5942	-0.0904	0.47192	-2.0438	2.099	-0.043	0.22478	-0.9735	1	0.09756	0.11235	11.401
8	O4	-1.5836	0.35372	-0.022	1.70826	1.745	0.20275	-0.0126	0.97915	1	0.09756	0.12369	16.9516
				Cell Volume		577			Dipole Moment			Magnitude	
				Z		2			x	y	z		
				Total Dipole Moment =			0.00606	esu*cm/A^3	0.9447	1.3899	0.4832	1.7486	debye

TeO3 in CTW			Coord.			distance	x	y	z	unitized	C_grav	C_charge	u_debye
Z		charges	x	y	z								
52	Te	3.539370714	0	0	6.411452								
8	O3	-1.17979024	-0.97901	0.940902	5.520097	1.624275497	-0.60274	-0.57927	-0.548770822	1	0.133333	0.15926	11.17418
8	O3	-1.17979024	-0.9409	-1.91991	5.520097	2.316432808	-0.40618	0.828822	-0.384796398	1	0.133333	0.15926	15.93586
8	O3	-1.17979024	1.91991	0.979007	5.520097	2.332171274	0.823229	-0.41978	-0.382199631	1	0.133333	0.15926	16.04414
				Cell Volume		577				Dipole Moment		Magnitude	
				Z		2				x	y	z	
				Total Dipole Moment =		0.0638	esu*cm/A^3			-1.77636E-15	6.87948E-06	-18.3962	**18.3962**	esu*cm
					pm/V	152,206,931.92	ion to pm/V cm/A^3						

TeO3 in CTW			Coord.			distance	x	y	z	unitized	C_grav	C_charge	u_debye
Z		charges	x	y	z								
52	Te	3.539370714	0	0	0								
8	O3	-1.17979024	-0.97901	0.940902	-0.89136	1.624275497	-0.60274	0.579275	-0.548770822	1	0.133333	0.15926	11.17418
8	O3	-1.17979024	-0.9409	-1.91991	-0.89136	2.316432808	-0.40618	-0.82882	-0.384796398	1	0.133333	0.15926	15.93586
8	O3	-1.17979024	1.91991	0.979007	-0.89136	2.332171274	0.823229	0.419783	-0.382199631	1	0.133333	0.15926	16.04414
2	Lp	-2	0	4.594E-07	1.228456	1.228456269	0	3.74E-07	1	1	0.037037	0.076248	11.20453
				Cell Volume		577				Dipole Moment		Magnitude	
				Z		2			x	y	z		
				Total Dipole Moment =		0.02493	esu*cm/A^3		-1.77636E-15	-2.68941E-06	-7.19166	7.1917	esu*cm
					pm/V	59,502,545.49	ion to pm/V cm/A^3						

Figure S4. Bond valence calculation for $Cs_2TeW_3O_{12}$.

Bond valence calculation for $Cs_2TeW_3O_{12}$		
	bond-distance	bond valence
Cs1		
Cs1-O4	3.028	0.159558275
Cs1-O4	3.028	0.159558275
Cs1-O4	3.028	0.159558275
Cs1-O2	3.094	0.136304495
Cs1-O2	3.094	0.136304495
Cs1-O2	3.094	0.136304495
Cs1-O1	3.41	0.064117331
Cs1-O1	3.41	0.064117331
Cs1-O1	3.41	0.064117331
Cs1-O3	3.673	0.034227511
Cs1-O3	3.673	0.034227511
Cs1-O3	3.673	0.034227511
$\sum S_i$		**1.182622838**
Cs2		
Cs2-O3	3.113	0.130261668
Cs2-O3	3.113	0.130261668
Cs2-O3	3.113	0.130261668
Cs2-O1	3.495	0.052344703
Cs2-O1	3.495	0.052344703
Cs2-O1	3.495	0.052344703
Cs2-O2	3.675	0.034064523
Cs2-O2	3.675	0.034064523
Cs2-O2	3.675	0.034064523
Cs2-O4	3.74	0.029169546
Cs2-O4	3.74	0.029169546
Cs2-O4	3.74	0.029169546
$\sum S_i$		**0.737521318**
W		
W-O1	1.8302	0.78238729
W-O2	2.0442	1.395109592
W-O3	2.0288	1.338234692
W-O4	1.8467	0.818067186
W-O5	2.1096	1.664841177
W-O6	1.7469	0.624664521
$\sum S_i$		**6.623304458**
Te		
Te1-O3	1.8866	1.179790238
Te1-O3	1.8866	1.179790238
Te1-O3	1.8866	1.179790238
$\sum S_i$		**3.539370714**