Electronic Supplementary Information for:

Characterization and Optimization of the Growth Conditions of a

Novel Cs₂TeW₃O₁₂ Piezoelectric Crystal

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Fig. S1 Ball-and-stick diagram of CTW in ac-plane.

Fig. S2 Directions of dipole moments of each WO₆ and TeO₃ polyhedra in the unit cell of CTW.

Fig. S3 Atomic coordinates and dipole moment of CTW.

Fig. S4. Bond valence calculation for Cs₂TeW₃O₁₂.

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 WO₆ octahedra, and TeO₃ 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.



Atomic coordinates for Cs ₂ TeW ₃ O ₁₂							
	x	у	Z	x	у	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	
Те	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	

Figure S3. Atomic coordinates and dipole moment of CTW.

WO ₆ in CTW C			art. Coor	d.	distance	istance unit				dipole moment for each			
Z	atom	charges	x	у	z	Å	x	у	z	unitized Vec	C_grav	C_charge	u_debye
74	W	6.09979	6.25854	8.74072	3.47633								
8	01	-1.264	8.25635	9.15475	3.35747	2.044	-0.9775	-0.2026	0.05816	1	0.09756	0.12006	17.0313
8	01	-0.709	5.50106	6.4295	3.35747	2.435	0.31107	0.94913	0.04881	1	0.09756	0.11368	14.4353
8	02	-0.739	4.01789	7.97495	3.95055	2.415	0.92784	0.3171	-0.1964	1	0.09756	0.11403	14.6309
8	02	-1.209	6.68085	10.6987	3.95055	2.058	-0.2052	-0.9512	-0.2304	1	0.09756	0.11943	16.662
8	03	-0.594	6.34889	8.2688	5.5201	2.099	-0.043	0.22478	-0.9735	1	0.09756	0.11235	11.401
8	04	-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 5		577			Dipole Momen		t Magnitude		
				2	Z	2			х	у	Z		
				Total D	ipole Mo	oment = 0.00606 as		esu*cm/A^3	0.9447	1.3899	0.4832	1.7486	debye
			Cart. Coord.			unit vector				dipole moment for each			
V	VO ₆ in CT	W	0	art. Coor	d.	distance		unit	vector		dipole	moment f	or each
Z	VO ₆ in CT atom	W charges	x	art. Coor y	d. z	distance Å	x	unit y	vector z	unitized Vec	dipole C_grav	moment fo C_charge	or each u_debye
Z 74	VO ₆ in CT atom W	W charges 6.09979	x 0	Cart. Coor y 0	d. z	distance Å	x	unit y	vector z	unitized Vec	dipole C_grav	moment fo C_charge	or each u_debye
Z 74 8	VO ₆ in CT atom W O1	w charges 6.09979 -1.2644	x 0 -1.9978	y 0 -0.414	d. z 0 0.11886	distance Å 2.044	x -0.9775	unit y -0.2026	vector z 0.05816	unitized Vec	dipole C_grav 0.09756	moment fo C_charge 0.12006	or each u_debye 17.0313
Z 74 8 8	VO ₆ in CT atom W O1 O1	charges 6.09979 -1.2644 -0.7091	x 0 -1.9978 0.75749	2art. Coor y 0 -0.414 2.31122	d. z 0.11886 0.11886	distance Å 2.044 2.435	x -0.9775 0.31107	unit y -0.2026 0.94913	z 0.05816 0.04881	unitized Vec	dipole C_grav 0.09756 0.09756	moment fo C_charge 0.12006 0.11368	or each u_debye 17.0313 14.4353
Z 74 8 8 8 8	VO ₆ in CT atom W O1 O1 O2	charges 6.09979 -1.2644 -0.7091 -0.7392	x 0 -1.9978 0.75749 2.24065	2art. Coord y 0 -0.414 2.31122 0.76577	d. 2 0 0.11886 0.11886 -0.4742	distance Å 2.044 2.435 2.415	x -0.9775 0.31107 0.92784	unit y -0.2026 0.94913 0.3171	z 0.05816 0.04881 -0.1964	unitized Vec	dipole C_grav 0.09756 0.09756 0.09756	moment fo C_charge 0.12006 0.11368 0.11403	or each u_debye 17.0313 14.4353 14.6309
Z 74 8 8 8 8 8	VO ₆ in CT atom W O1 O1 O2 O2 O2	charges 6.09979 -1.2644 -0.7091 -0.7392 -1.2092	x 0 -1.9978 0.75749 2.24065 -0.4223	y 0 -0.414 2.31122 0.76577 -1.958	d. 2 0 0.11886 0.11886 -0.4742 -0.4742	distance Â 2.044 2.435 2.415 2.058	x -0.9775 0.31107 0.92784 -0.2052	unit y -0.2026 0.94913 0.3171 -0.9512	z 0.05816 0.04881 -0.1964 -0.2304	unitized Vec 1 1 1 1	dipole C_grav 0.09756 0.09756 0.09756 0.09756	moment fo C_charge 0.12006 0.11368 0.11403 0.11943	u_debye 17.0313 14.4353 14.6309 16.662
Z 74 8 8 8 8 8 8 8	VO ₆ in CT atom W O1 O1 O2 O2 O2 O3	charges 6.09979 -1.2644 -0.7091 -0.7392 -1.2092 -0.5942	x 0 -1.9978 0.75749 2.24065 -0.4223 -0.0904	y 0 -0.414 2.31122 0.76577 -1.958 0.47192	d. 2 0 0.11886 0.11886 -0.4742 -0.4742 -2.0438	A 2.044 2.435 2.415 2.058 2.099	x -0.9775 0.31107 0.92784 -0.2052 -0.043	unit y -0.2026 0.94913 0.3171 -0.9512 0.22478	z 0.05816 0.04881 -0.1964 -0.2304 -0.9735	unitized Vec 1 1 1 1 1 1 1 1	dipole C_grav 0.09756 0.09756 0.09756 0.09756 0.09756	moment for C_charge 0.12006 0.11368 0.11403 0.11943 0.11235	r each u_debye 17.0313 14.4353 14.6309 16.662 11.401
Z 74 8 8 8 8 8 8 8 8 8	VO ₆ in CT atom W O1 O1 O2 O2 O3 O4	charges 6.09979 -1.2644 -0.7091 -0.7392 -1.2092 -0.5942 -1.5836	x 0 -1.9978 0.75749 2.24065 -0.4223 -0.0904 0.35372	y 0 -0.414 2.31122 0.76577 -1.958 0.47192 -0.022	d. 2 0 0.11886 0.11886 -0.4742 -0.4742 -2.0438 1.70826	A 2.044 2.435 2.415 2.058 2.099 1.745	x -0.9775 0.31107 0.92784 -0.2052 -0.043 0.20275	vnit y -0.2026 0.94913 0.3171 -0.9512 0.22478 -0.0126	z 0.05816 0.04881 -0.1964 -0.2304 -0.9735 0.97915	unitized Vec 1 1 1 1 1 1 1 1	dipole C_grav 0.09756 0.09756 0.09756 0.09756 0.09756 0.09756	moment for C_charge 0.12006 0.11368 0.11403 0.11943 0.11235 0.12369	v_each v_debye 17.0313 14.4353 14.6309 16.662 11.401 16.9516
Z 74 8 8 8 8 8 8 8	WO ₆ in CT atom W O1 O2 O2 O3 O4	charges 6.09979 -1.2644 -0.7091 -0.7392 -1.2092 -0.5942 -1.5836	x 0 -1.9978 0.75749 2.24065 -0.4223 -0.0904 0.35372	vart. Coord y 0 -0.414 2.31122 0.76577 -1.958 0.47192 -0.022 Cell V	d. 2 0 0.11886 0.11886 -0.4742 -0.4742 -2.0438 1.70826 ohume	A 2.044 2.435 2.415 2.058 2.099 1.745 577	x -0.9775 0.31107 0.92784 -0.2052 -0.043 0.20275	y -0.2026 0.94913 0.3171 -0.9512 0.22478 -0.0126	z 0.05816 0.04881 -0.1964 -0.2304 -0.9735 0.97915	unitized Vec 1 1 1 1 1 1 Dipole Momen	dipole C_grav 0.09756 0.09756 0.09756 0.09756 0.09756 0.09756 t	moment fo C_charge 0.12006 0.11368 0.11403 0.11943 0.11235 0.12369 Magnitude	r each a_debye 17.0313 14.4353 14.6309 16.662 11.401 16.9516
Z 74 8 8 8 8 8 8 8 8	VO ₆ in CT atom W O1 O1 O2 O2 O3 O4	charges 6.09979 -1.2644 -0.7091 -0.7392 -1.2092 -0.5942 -1.5836	x 0 -1.9978 0.75749 2.24065 -0.4223 -0.0904 0.35372	vart. Coord y 0 -0.414 2.31122 0.76577 -1.958 0.47192 -0.022 Cell V 2	d. 2 0 0.11886 0.11886 -0.4742 -0.4742 -2.0438 1.70826 Yohume Z	A 2.044 2.435 2.415 2.058 2.099 1.745 577 2	x -0.9775 0.31107 0.92784 -0.2052 -0.043 0.20275	vnit y -0.2026 0.94913 0.3171 -0.9512 0.22478 -0.0126	z 0.05816 0.04881 -0.1964 -0.2304 -0.9735 0.97915 x	unitized Vec 1 1 1 1 1 1 Dipole Momen y	dipole C_grav 0.09756 0.09756 0.09756 0.09756 0.09756 0.09756 t z	moment fo C_charge 0.12006 0.11368 0.11403 0.11943 0.11235 0.12369 Magnitude	or each u_debye 17.0313 14.4353 14.6309 16.662 11.401 16.9516

	TeO3 in CT	W		Coord.									
Z		charges	x	у	z	distance	x	у	z	unitized	C_grav	C_charge	u_debye
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	e:	577				Dipole Moment		Magnitude	
				Z		2			х	у	z		
			Total	Dipole Mon	ient =	0.0638	esu*cm/A^3	3	-1.77636E-15	6.87948E-06	-18.3962	18.3962	esu*cm
					pm/V	152,206,931.92	ion to pm/	/ cm/A^3					
	TeO3 in CT	W		Coord.									
Z		charges	x	у	z	distance	x	У	z	unitized	C_grav	C_charge	u_debye
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	t	Magnitude	
				Z		2			x	У	z		
			Total	Dipole Mon	nent =	0.02493	esu*cm/AA	3	-1.77636E-15	-2.68941E-06	-7.19166	7.1917	esu*cm
					pm/V	59,502,545.49	ion to pm/\	/ cm/A^3					

Figure S4. Bond valence calculation for Cs₂TeW₃O₁₂.

	Bond	valence	calculation	for	Cs ₂ TeW ₃	O 12
- 1						

	bond-distance	bond valence
Cs1		
Cs1-04	3.028	0.159558275
Cs1-04	3.028	0.159558275
Cs1-04	3.028	0. 159558275
Cs1-02	3.094	0.136304495
Cs1-02	3.094	0.136304495
Cs1-02	3.094	0.136304495
Cs1-01	3.41	0.064117331
Cs1-01	3.41	0.064117331
Cs1-01	3.41	0.064117331
Cs1-03	3.673	0.034227511
Cs1-03	3.673	0.034227511
Cs1-03	3.673	0.034227511
Σs_i		1. 182622838
Cs2		
Cs2-03	3.113	0. 130261668
Cs2-03	3.113	0. 130261668
Cs2-03	3. 113	0. 130261668
Cs2-01	3.495	0.052344703
Cs2-01	3.495	0.052344703
Cs2-01	3.495	0.052344703
Cs2-02	3.675	0. 034064523
s2-02	3.675	0.034064523
s2-02	3.675	0.034064523
s2-04	3.74	0.029169546
s2-04	3.74	0.029169546
s2-04	3.74	0.029169546
ΣS_i		0.737521318
I		
-01	1.8302	0.78238729
-02	2.0442	1.395109592
-03	2.0288	1.338234692
-04	1.8467	0.818067186
-05	2.1096	1.664841177
-06	1.7469	0.624664521
ΣS_i		6. 623304458
`e		
e1-03	1. 8866	1. 179790238
e1-03	1. 8866	1. 179790238
'e1-03	1. 8866	1. 179790238
Σc	1.0000	3 539370714