

Electronic Supplementary Information

Electric-elastic properties of a novel high-quality CdTeMoO₆ piezoelectric crystal

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Table S1. The direction and magnitude of the dipole moments of the TeO₄, MoO₄ polyhedrons in CdTM crystal.

Dipole moment					
Species	x(a)	y(b)	z(c)	Magnitude	
				debye	esu·cm/Å ³
TeO ₄	0	0	11.9907	11.9907	0.0948
MoO ₄	0	0	-6.9996	6.9996	0.0554
Asymmetric unit	0	0	4.9911	4.9911	0.0395
Unit cell	0	0	0	0	0

Table S2. Local dipole moment calculation for MoO₄ and TeO₄.

Mo ₄ in CdTM			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	
42	Mo1	5.592961187	0	0	0									
8	O2	-1.1143669	-1.1474676	1.1474676	0.92376895	1.867274179	-0.61451479	0.61451479	0.494715217	1	0.16	0.200221561	16.41057936	
8	O2	-1.1143669	1.1474676	-1.1474676	0.92376895	1.867274179	0.61451479	-0.61451479	0.494715217	1	0.16	0.200221561	16.41057936	
8	O3	-1.68211369	-0.9514683	-0.9514683	-1.04881075	1.706044502	-0.55770427	-0.55770427	-0.61476166	1	0.16	0.210073589	18.89900923	
8	O3	-1.68211369	0.9514683	0.9514683	-1.04881075	1.706044502	0.557704268	0.557704268	-0.61476166	1	0.16	0.210073589	18.89900923	
			Cell Volume			252.893316				Dipole Moment			Magnitude	
			Z			2				x	y	z		
			Total Dipole Moment =	0.055356512		esu*cm/Å ³	0			0	0	-6.99964593	6.9996459	debye
TeO ₄ in CdTM			Cart. Coord.			distance	unit vector			dipole moment for each				
Z		charges	x	y	z	Å	x	y	z	unitized	C_grav	C_charge	u_debye	
52	Te(1)	3.719920153	0	0	0									
8	O1	-1.25130815	1.0069398	1.0069398	-1.20094494	1.862826957	0.540543928	0.540543928	-0.64468948	1	0.133333333	0.160804536	13.51702892	
8	O1	-1.25130815	-1.0069398	-1.0069398	-1.20094494	1.862826957	-0.54054393	-0.54054393	-0.64468948	1	0.133333333	0.160804536	13.51702892	
8	O2	-0.60865192	1.4940324	-1.4940324	-0.41173184	2.152623686	0.694051826	-0.69405183	-0.19126977	1	0.133333333	0.151324378	10.34899276	
8	O2	-0.60865192	-1.4940324	1.4940324	-0.41173184	2.152623686	-0.69405183	0.694051826	-0.19126977	1	0.133333333	0.151324378	10.34899276	
2	Lp	-2	0	0	1.027205687	1.027205687	0	0	1	1	0.037037037	0.076510977	9.396737851	
			Cell Volume			252.893316				Dipole Moment			Magnitude	
			Z			2				x	y	z		
			Total Dipole Moment =	0.094828396		esu*cm/Å ³	0			0	0	-11.9907338	11.990734	debye