

Supporting information

Piezoelectricity and Related Properties in Orthorhombic Cadmium Diiodate

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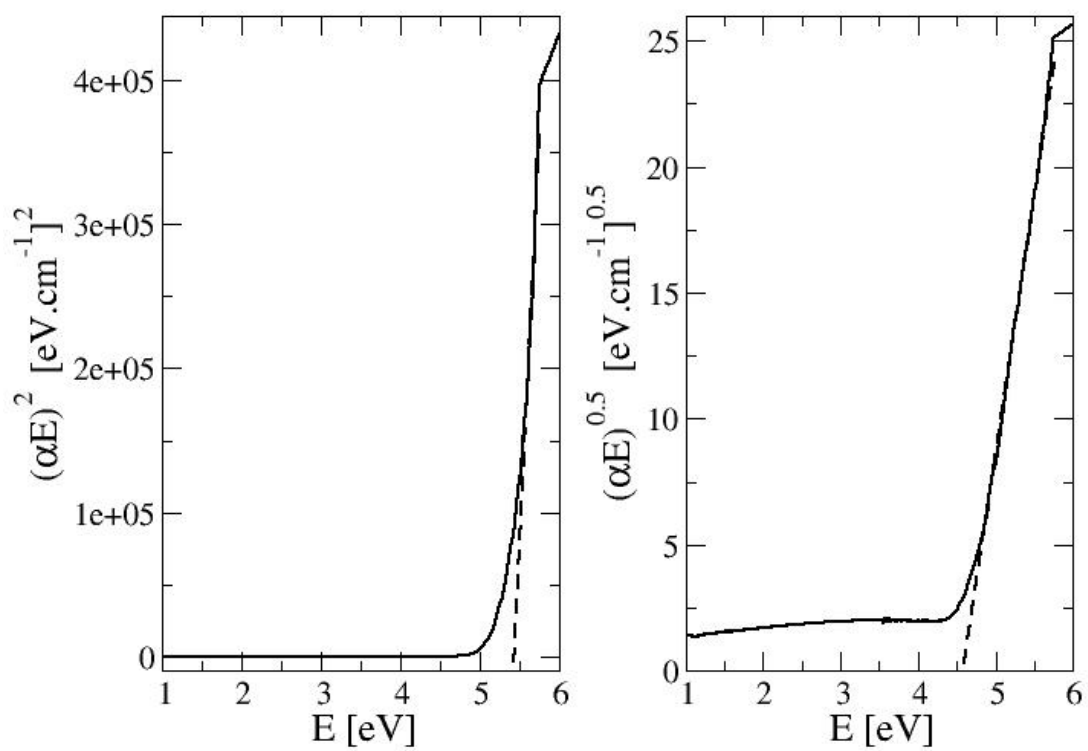


Figure S1. $(\alpha E)^2$ and $(\alpha E)^{\frac{1}{2}}$ Tauc plots of CDI obtained from UV-vis spectroscopy.

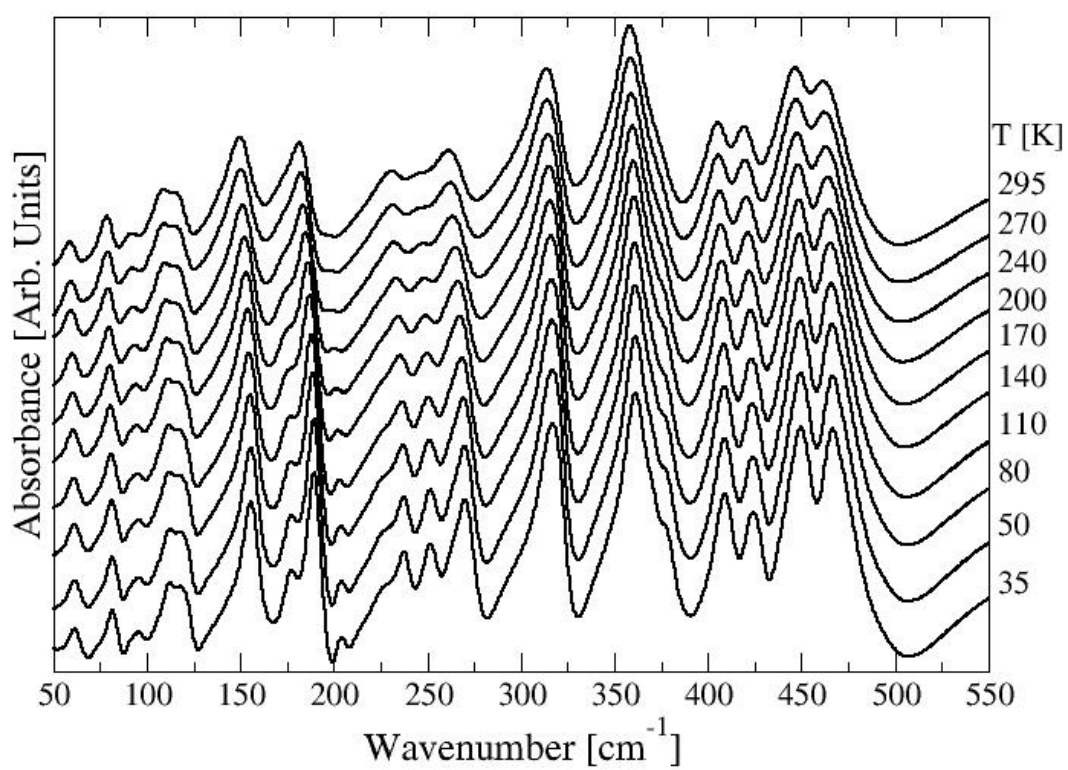


Figure S2. Experimental far-infrared (50–550 cm^{-1}) signatures of CDI between 35 and 295 K.

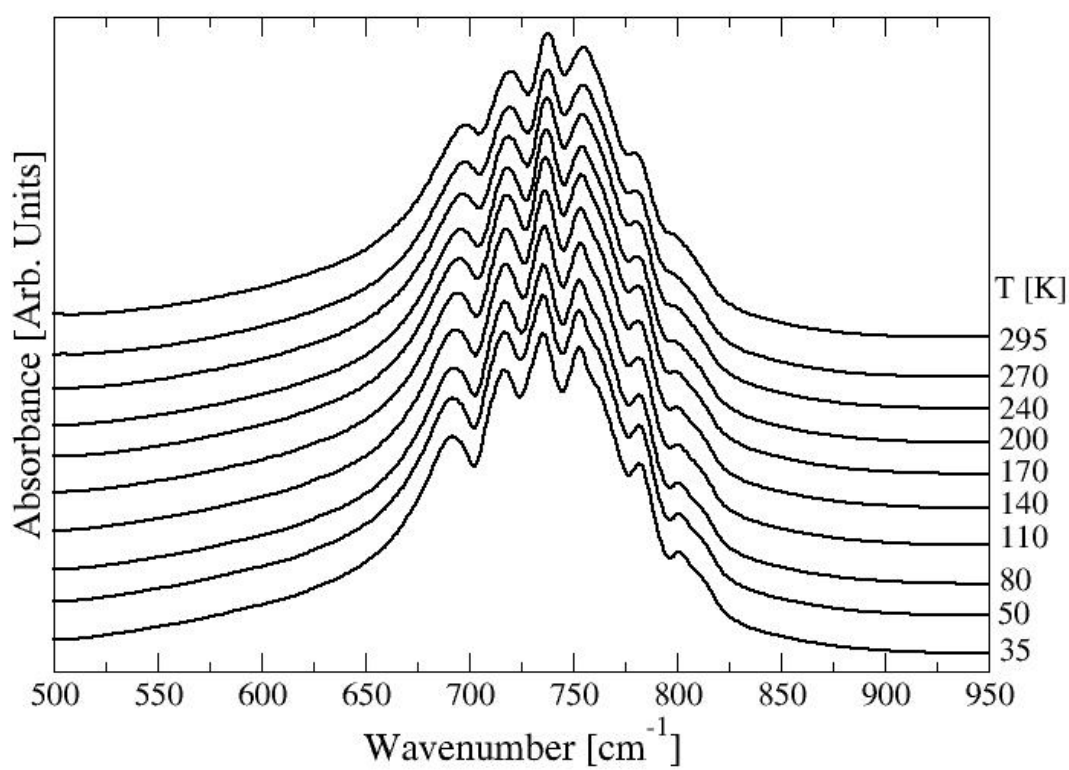


Figure S3. Experimental mid-infrared (500–950 cm^{-1}) signatures of CDI between 35 and 295 K.

Tables S1. Refinement details of CDI single crystal from x-ray diffraction.

Formula mass (amu)	462.231	$2\theta_{max}$ ($^{\circ}$)	93.71
Color and habit	colorless	ρ_{calc} ($\text{g}\cdot\text{cm}^{-3}$)	5.36
Crystal system	Orthorhombic	λ (\AA)	0.71073
Space group	$P2_12_12_1$	μ ($\text{Mo K}\alpha$) (cm^{-1})	150.13
a (\AA)	5.856(10)	Reflections collected	150137
b (\AA)	17.480(3)	Independent reflection	4614
c (\AA)	5.588(10)	Restraints/Parameters	0/82
Ω (\AA^3)	572.00(17)	R(F) for $F_0^2 > 2\sigma(F_0^2)$	0.3095
Z	4	Rw(F_0^2)	0.0176
T ($^{\circ}\text{C}$)	23	Flack factor	0.125
$2\theta_{min}$ ($^{\circ}$)	4.56	R1	0.0175

atom	x/a	y/b	z/c
I	0.63731(2)	0.42249(2)	0.52928(3)
I	0.21388(2)	0.29137(2)	0.75431(3)
Cd	0.17159(3)	0.40658(2)	0.20690(3)
O	0.5053(3)	0.33882(12)	0.3893(4)
O	0.0211(3)	0.33677(13)	0.5412(4)
O	0.0299(4)	0.29231(13)	1.0153(4)
O	0.8161(3)	0.45290(13)	0.2793(4)
O	0.3712(4)	0.37540(12)	0.8613(4)
O	0.3955(3)	0.48426(11)	0.48426(11)

Table S2. Calculated zone-center transverse optical (TO) frequencies (in cm^{-1}) of CDI using the PBEvdW model with their symmetries.

Sym.	Freq.	Sym.	Freq.	Sym.	Freq.	Sym.	Freq.	Sym.	Freq.
A	37	B ₁	130	B ₃	222	B ₃	408	B ₁	674
B ₂	39	A	135	A	233	A	416	A	689
B ₂	41	B ₁	142	B ₃	237	B ₁	420	B ₁	691
A	42	B ₃	146	B ₁	252	B ₂	427	B ₃	698
B ₁	59	A	148	B ₂	254	A	430	A	701
B ₃	63	B ₃	152	A	256	B ₃	431	B ₂	707
B ₃	65	A	152	B ₃	262	B ₁	436	B ₃	711
A	68	B ₂	153	B ₁	263	B ₂	443	B ₂	721
B ₁	77	B ₁	154	B ₂	265	B ₃	450	B ₁	724
A	78	B ₂	163	B ₂	283	B ₂	560		
B ₃	79	B ₁	170	B ₁	290	A	577		
B ₁	84	B ₃	171	A	292	B ₁	593		
B ₁	90	B ₂	178	B ₃	298	B ₃	598		
B ₂	93	A	179	A	325	B ₁	619		
B ₃	95	B ₁	185	B ₃	327	B ₃	622		
A	98	B ₁	185	A	332	A	623		
B ₃	104	B ₂	186	B ₂	333	B ₂	626		
A	107	B ₂	189	B ₁	337	B ₂	630		
B ₁	109	B ₃	193	B ₃	344	A	640		
B ₂	112	B ₃	200	B ₁	351	B ₂	641		
B ₂	115	A	201	B ₂	355	B ₁	643		
B ₃	116	A	218	A	383	B ₃	649		
A	119	B ₂	220	B ₁	384	A	665		
B ₂	125	B ₁	221	B ₂	401	B ₃	666		