Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information

Combination of Multiple Chromophores Enhances Second-Harmonic Generation in Nonpolar Noncentrosymmetric Oxide: $CdTeMoO_6$

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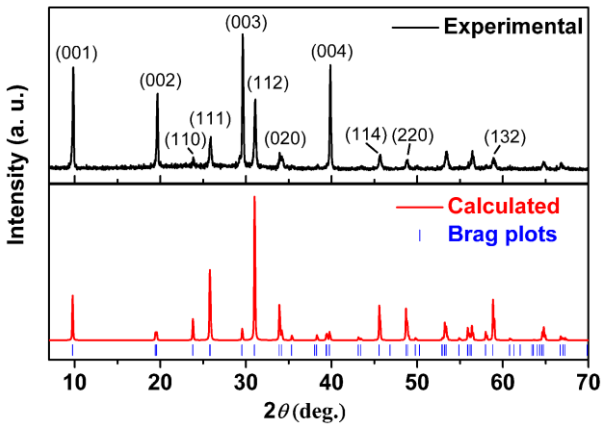

Figure S1. Experimental and calculated PXRD patterns for $CdTeMoO_6$.

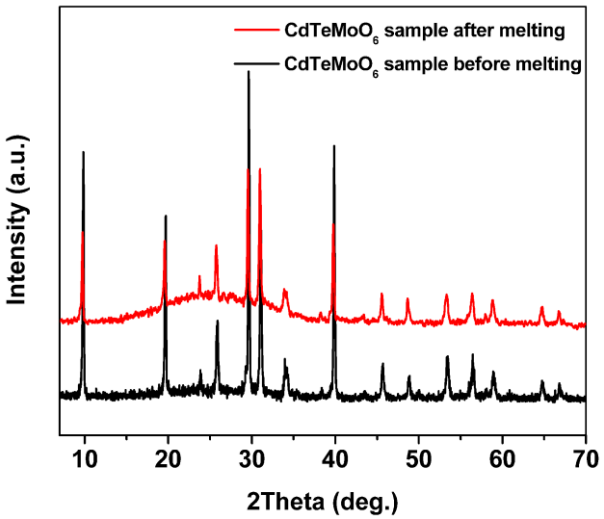

Figure S2. PXRD patterns of $CdTeMoO_6$ powders before and after melting.

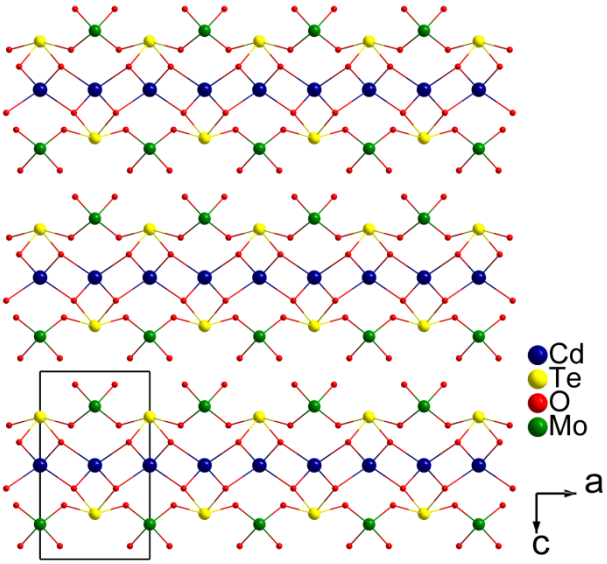

Figure S3. The neutral layered structure of $CdTeMoO_6$.

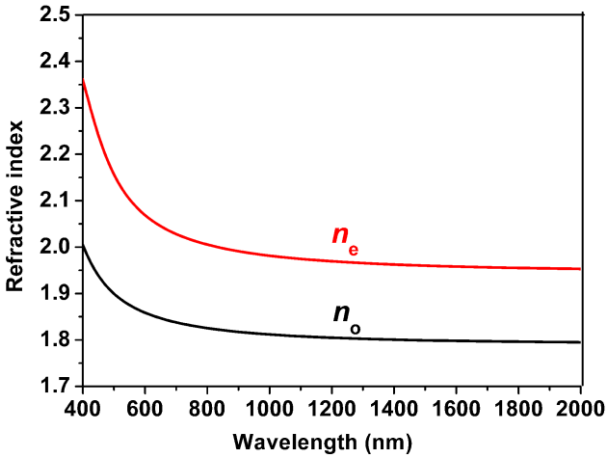

Figure S4. Calculated linear refractive indices for $CdTeMoO_6$.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $CdTeMoO_6$.

Atom	*Wyck.*	*x/a*	*y/b*	*z/c*	U_{eq} [$Å^2$][a]
Cd	2b	1/2	1/2	1/2	0.0094(1)
Te	2c	1	1/2	0.24243(4)	0.0074(1)
Mo	2c	1/2	0	0.18599(6)	0.0081(1)
O1	4e	0.1910(6)	0.3090(6)	0.3769(4)	0.0137(8)
O2	4e	0.3197(5)	0.1803(5)	0.0701(5)	0.0161(9)
O3	4e	0.7179(5)	0.2179(5)	0.2872(5)	0.0125(8)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond distances (Å) and angles (deg.) for $CdTeMoO_6$.

Cd—O1	2.221(2)	Te—$O3^{v}$	2.148(4)
Cd—$O1^{i}$	2.221(2)	Te—O3	2.148(4)
Cd—$O1^{ii}$	2.221(2)	Mo—O2	1.709(4)
Cd—$O1^{iii}$	2.221(2)	Mo—O3	1.869(4)
Te—$O1^{iv}$	1.877(4)	Mo—$O2^{viii}$	1.709(4)
Te—$O1^{i}$	1.877(4)	Mo—$O3^{viii}$	1.869(4)
O1—Cd—$O1^{i}$	119.65(18)	$O1^{iv}$—Te—O3	82.95(8)
O1—Cd—$O1^{ii}$	104.63(8)	$O1^{i}$—Te—O3	82.95(8)
$O1^{i}$—Cd—$O1^{ii}$	104.63(8)	$O3^{v}$—Te—O3	158.2(2)
O1—Cd—$O1^{iii}$	104.63(8)	$O2^{viii}$—Mo—O2	104.1(3)
$O1^{i}$—Cd—$O1^{iii}$	104.63(8)	$O2^{viii}$—Mo—O3	107.57(9)
$O1^{ii}$—Cd—$O1^{iii}$	119.65(18)	O2—Mo—O3	107.57(9)
$O1^{iv}$—Te—$O1^{i}$	99.0(3)	$O2^{viii}$—Mo—$O3^{viii}$	107.57(9)
$O1^{iv}$—Te—$O3^{v}$	82.95(8)	O2—Mo—$O3^{viii}$	107.57(9)
$O1^{i}$—Te—$O3^{v}$	82.95(8)	O3—Mo—$O3^{viii}$	121.2(2)

Symmetry codes: (i) 1-x, 1-y, z; (ii) 1-y, x, 1-z; (iii) y, 1-x, 1-z; (iv) 1+x, y, z; (v) 2-x, 1-y, z; (vi) -1+x, y, z; (vii) -0.5+x, 0.5-y, 1-z; (viii) 1-x, -y, z.

Table S3. Anisotropic displacement parameters ($Å^2$) for $CdTeMoO_6$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd	0.00836(18)	0.00836(18)	0.0116(2)	0	0	0
Te	0.00848(16)	0.00848(16)	0.0053(2)	0.0009(4)	0	0
Mo	0.00856(18)	0.00856(18)	0.0072(3)	-0.0029(6)	0	0
O1	0.0137(11)	0.0137(11)	0.014(2)	-0.0032(18)	-0.0077(12)	0.0077(12)
O2	0.0184(13)	0.0184(13)	0.011(2)	0.0037(17)	-0.0030(14)	0.0030(14)
O3	0.0121(12)	0.0121(12)	0.013(2)	-0.0046(17)	-0.0015(13)	-0.0015(13)