Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

$ZnTeMoO_6$: A strong second-harmonic generation material originating from three types of asymmetric building units

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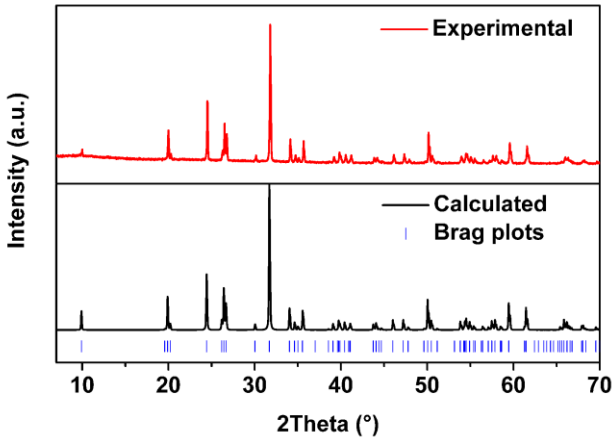

Figure S1. Experimental and calculated PXRD patterns for $ZnTeMoO_6$.

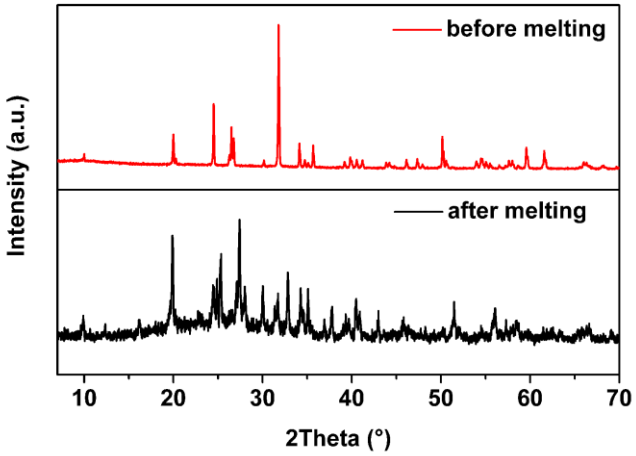

Figure S2. XRD patterns of $ZnTeMoO_6$ before and after melting.

Figure S3. Photograph of the volatile matter.

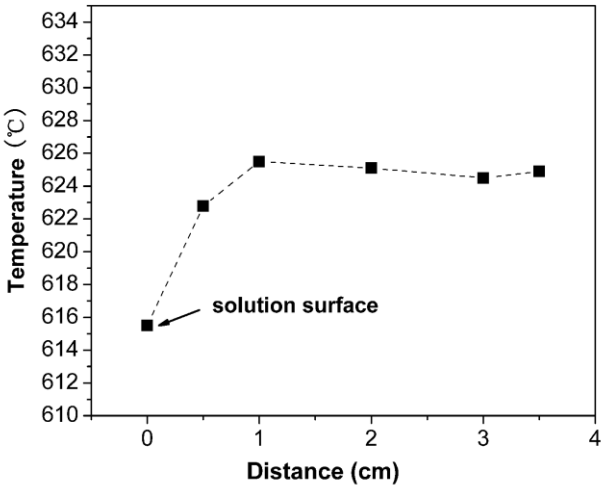

Figure S4. The representative temperature gradient in the vertical direction of the furnace.

Table S1. Selected bond distances (Å) and angles (deg) for $ZnTeMoO_6$.

Zn—O1^{i}	2.05(1)	O1^{i}—Zn—O2	167.2(4)
Zn—O1^{ii}	2.05(1)	O1^{ii}—Zn—O2	82.9(4)
Zn—O1^{iii}	2.186(9)	O1^{iii}—Zn—O2	71.9(3)
Zn—O1	2.186(9)	O1—Zn—O2	78.3(4)
Zn—O2	2.269(10)	O1^{i}—Zn—O2^{iii}	82.9(4)
Zn—O2^{iii}	2.269(10)	O1^{ii}—Zn—O2^{iii}	167.2(4)
Mo—O3^{iv}	1.729(10)	O1^{iii}—Zn—O2^{iii}	78.3(4)
Mo—O3	1.729(10)	O1—Zn—O2^{iii}	71.9(3)
Mo—O2	1.843(9)	O2—Zn—O2^{iii}	84.9(5)
Mo—O2^{iv}	1.843(9)	O3^{iv}—Mo—O3	104.4(7)
Te—O1^{v}	1.888(10)	O3^{iv}—Mo—O2	106.1(4)
Te—O1	1.888(10)	O3—Mo—O2	108.0(4)
Te—O2^{iii}	2.097(9)	O3^{iv}—Mo—O2^{iv}	108.0(4)
Te—O2^{vi}	2.097(9)	O1^{v}—Te—O1	100.2(7)
		O1^{v}—Te—O2^{iii}	87.6(4)
		O1—Te—O2^{iii}	81.9(4)
		O1^{v}—Te—O2^{vi}	81.9(4)
		O1—Te—O2^{vi}	87.6(4)
		O2^{iii}—Te—O2^{vi}	163.7(5)

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

Table S2. Anisotropic displacement parameters ($Å^2$) for $ZnTeMoO_6$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn	0.0131(9)	0.0130(9)	0.0158(9)	-0.0019(12)	0.00000	0.00000
Mo	0.0109(6)	0.0119(7)	0.0158(7)	0.0027(9)	0.00000	0.00000
Te	0.0105(5)	0.0101(5)	0.0127(6)	0.0003(6)	0.00000	0.00000
O1	0.019(5)	0.014(4)	0.030(5)	0.008(4)	0.007(5)	0.005(4)
O2	0.019(5)	0.009(4)	0.018(4)	-0.001(3)	0.005(5)	-0.002(4)
O3	0.022(5)	0.023(5)	0.023(5)	-0.001(4)	0.008(5)	-0.001(5)