

Supporting Information for:

MgTeMoO₆: A Neutral Layered Material Showing Strong Second-harmonic Generation

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for MgTeMoO₆.

Fig. S1. Powder X-ray diffraction pattern of the residue of MgTeMoO₆ after differential scanning calorimetry and thermogravimetric analysis measurements.

Fig. S2. The theoretical morphology of MgTeMoO₆ established by using the Mercury program with its structural parameters according to the Bravais-Friedel and Donnay-Harker (BFDH) methods.

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Atom	x	y	z	U(eq)
Te	0	0	2433(1)	7(1)
Mo	0	0	6913(1)	8(1)
Mg	0	5000	309(2)	9(1)
O(1)	2219(5)	1697(5)	1058(3)	11(1)
O(2)	2351(5)	6741(6)	2052(3)	11(1)
O(3)	3539(6)	2854(5)	4250(3)	15(1)

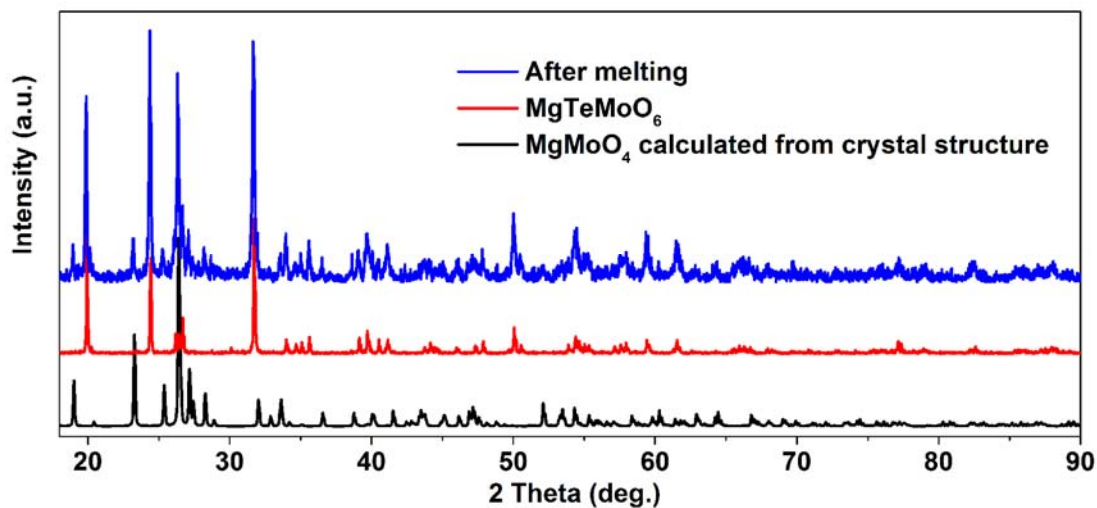


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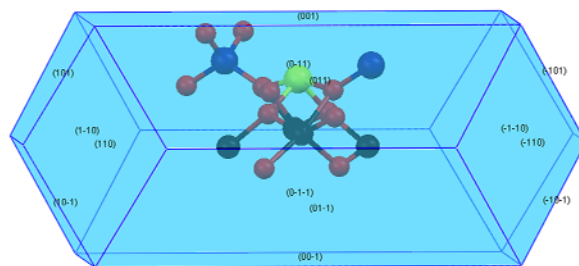


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