

Optical Anisotropy in Mo–Te–O Frameworks Constructed from Distorted MoO₆ and TeO₃ Units

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Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ and $\beta\text{-MoTe}_2\text{O}_7$. Ueq is defined as 1/3 of the trace of the orthogonalised UIJ tensor.

Compound	Atom	x	y	z	U(eq)
$(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$	Te1	6396.7(3)	4882.2(3)	3833.7(4)	8.15(9)
	Mo1	4836.2(4)	2282.4(4)	4943.1(5)	6.05(10)
	Mo2	11529.8(4)	2610.7(4)	2883.7(6)	9.50(11)
	Mg1	10000	5000	5000	2.2(4)
	O1	5945(3)	3828(3)	5635(5)	10.7(7)
	O2	6800(3)	6275(3)	5495(5)	9.0(7)
	O3	8092(3)	4230(4)	4340(5)	17.1(8)
	O4	10417(3)	3711(3)	3286(5)	14.0(7)
	O5	11681(3)	3100(4)	767(5)	14.6(7)
	O6	10532(3)	1273(3)	2172(5)	13.9(7)
	O7	3270(3)	1511(3)	3567(5)	9.2(7)
	O8	4850(3)	2069(3)	7253(5)	10.4(7)
	O9	5986(3)	1187(3)	4844(5)	14.1(7)
	N1	8403(6)	1466(8)	3910(9)	51.4(19)
$\beta\text{-MoTe}_2\text{O}_7$	Te1	7174.2 (2)	14294.3 (5)	3325.6 (2)	8.99 (6)
	Te2	8792.7 (2)	9674.6 (5)	4840.8 (2)	8.56 (6)
	Te3	8361.7 (2)	519.2 (5)	7235.5 (2)	9.42 (6)
	Te4	9872.5 (2)	5216.3 (5)	8836.7 (2)	8.91 (6)
	Mo1	5614.8 (2)	9495.3 (6)	1677.5 (2)	7.95 (7)
	Mo2	6718.9 (2)	5277.6 (6)	5651.8 (2)	7.89 (7)
	O1	9503.7 (18)	11650 (5)	4298.8 (17)	11.1 (5)
	O2	8597.3 (19)	6646 (5)	4069.3 (18)	12.5 (6)
	O3	7606.8 (18)	11407 (6)	4228.6 (18)	13.6 (6)
	O4	7987.8 (18)	12951 (5)	2784.2 (17)	10.5 (5)
	O5	6122.2 (18)	12258 (6)	2559.6 (19)	15.3 (6)
	O6	4594.7 (19)	11000 (6)	1008.3 (18)	15.3 (6)
	O7	5295.9 (19)	7331 (6)	2358.7 (19)	14.9 (6)
O8	9120.3 (19)	8359 (5)	8638.5 (17)	12.4 (6)	
O9	9267.0 (18)	3337 (5)	9514.0 (17)	11.2 (5)	

	O10	9212.3 (19)	3570 (6)	7674.8 (17)	14.1 (6)
	O11	7741.4 (18)	1799 (5)	7982.4 (16)	9.5 (5)
	O12	7532.4 (19)	2331 (5)	6165.1 (17)	13.7 (6)
	O13	7490 (2)	7217 (6)	5380.1 (19)	15.9 (6)
	O14	6041.0 (19)	3947 (6)	4616.1 (18)	14.2 (6)

Table S2. Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$.

Compound	Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
$(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$	H1A	8198.11	1474.35	2684.45	62
	H1B	8806.31	2179.25	4377.35	62
	H1C	8950.51	828.05	4377.35	62
	H1D	7639.71	1379.15	4208.55	62

Table S3. Selected Bond lengths for $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ and $\beta\text{-MoTe}_2\text{O}_7$.

Compound	Atom-Atom	Length(Å)	Atom-Atom	Length(Å)
$(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$	Te1-O3	1.840(4)	Mo2-O5e	2.287(4)
	Te1-O2	1.914(3)	Mg1-O4	2.046(4)
	Te1-O1	1.954(3)	Mg1-O4d	2.046(4)
	Mo1-O9	1.706(3)	Mg1-O6e	2.078(4)
	Mo1-O8	1.775(3)	Mg1-O6f	2.078(4)
	Mo1-O7	1.840(3)	Mg1-O3	2.079(4)
	Mo1-O1	1.995(3)	N \cdots O9	2.878(4)
	Mo1-O8b	2.174(3)	N \cdots O6	2.965(4)
	Mo1-O2a	2.258(3)	N \cdots O1	2.976(4)
	Mo2-O6	1.755(4)	N \cdots O3	3.005(4)
	Mo2-O5	1.756(4)	N-H1D \cdots O9	1.969(4)
	Mo2-O4	1.758(3)	N-H1B \cdots O3	2.317(4)
	Mo2-O7c	2.099(3)	N-H1A \cdots O1	2.405(4)
	Mo2-O2d	2.153(3)		
a:1-X,1-Y,1-Z;b:+X,1/2-Y,-1/2+Z;c:1+X,+Y,+Z;d:2-X,1-Y,1-Z; e:+X,1/2-Y,1/2+Z;f:2-X,1/2+Y,1/2-Z				
$\beta\text{-MoTe}_2\text{O}_7$	Te1-O4	1.889(3)	Mo1-O6	1.713(3)
	Te1-O5	1.917(3)	Mo1-O7	1.716(3)
	Te1-O3	1.953(3)	Mo1-O5	1.901(3)
	Te2-O2	1.881(3)	Mo1-O1c	2.046(3)
	Te2-O1	1.898(3)	Mo1-O4c	2.151(3)
	Te2-O3	1.930(3)	Mo1-O2a	2.256(3)
	Te3-O11	1.890(3)	Mo2-O13	1.704(3)
	Te3-O12	1.929(3)	Mo2-O14	1.720(3)
	Te3-O10	1.948(3)	Mo2-O12	1.896(3)
	Te4-O8	1.891(3)	Mo2-O9d	2.090(3)
	Te4-O9	1.908(4)	Mo2-O11d	2.151(3)
	Te4-O10	1.927(3)	Mo2-O8b	2.222(3)
a:3/2-X,1/2+Y,1/2-Z;b:3/2-X,-1/2+Y,3/2-Z; c:3/2-X,-1/2+Y,1/2-Z; d:3/2-X,1/2+Y,3/2-Z				

Table S4. Selected Bond angles for $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ and $\beta\text{-MoTe}_2\text{O}_7$.

Compound	Atom-Atom-Atom	Angle(°)
$(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$	O2-Te1-O1	91.99(14)
	O3-Te1-O1	94.40(16)
	O3-Te1-O2	99.51(15)
	N1-H1A...O1	122.25(432)
	N1-H1B...O3	134.11(555)
	N1-H1D...O9	179.74(434)
$\beta\text{-MoTe}_2\text{O}_7$	O4-Te1-O3	88.54(12)
	O5-Te1-O3	93.80(11)
	O4-Te1-O5	94.70(12)
	O2-Te2-O1	95.19(12)
	O2-Te2-O3	97.34(12)
	O1-Te2-O3	98.59(12)
	O11-Te3-O10	87.26(12)
	O11-Te3-O12	94.12(12)
	O12-Te3-O10	95.82(12)
	O8-Te4-O9	95.19(12)
	O8-Te4-O10	96.21(12)
	O9-Te4-O10	97.99(11)

Table S5. Calculated bond valence sums (BVS) for atoms in $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ and $\beta\text{-MoTe}_2\text{O}_7$, obtained using the bond valence–bond length relation $s=\exp[(R_0-R)/B]$. R_0 and B parameters were taken from Brown’s bond valence parameter tables^[1].

Compound	Bond	d (Å)	s (v.u.)	Bond	d (Å)	s (v.u.)	
$(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$	Mo1-O1	1.995	0.788330518	Mo2-O2	2.154	0.512954789	
	Mo1-O2	2.258	0.387264	Mo2-O4	1.759	1.491824698	
	Mo1-O7	1.84	1.198512352	Mo2-O5	1.756	1.503969744	
	Mo1-O8	1.775	1.428688309	Mo2-O5	2.287	0.358069912	
	Mo1-O8	2.174	0.485963568	Mo2-O6	1.755	1.508040025	
	Mo1-O9	1.706	1.721581325	Mo2-O7	2.098	0.596774346	
	BVS of Mo1		6.010340071		BVS of Mo2		5.971633514
	Mg1-O3	2.079	0.352310199	Te1-O1	1.955	1.061262736	
	Mg1-O3	2.079	0.352310199	Te1-O2	1.913	1.188833974	
	Mg1-O4	2.046	0.385176328	Te1-O3	1.84	1.448125947	
	Mg1-O4	2.046	0.385176328				
	Mg1-O6	2.078	0.353263677				
	Mg1-O6	2.078	0.353263677				
	BVS of Mg1		2.181500409		BVS of Te1		3.698222657
$\beta\text{-MoTe}_2\text{O}_7$	Mo1-O6	1.713	1.689317032	Mo2-O13	1.704	1.730912366	
	Mo1-O7	1.716	1.675675246	Mo2-O14	1.72	1.657657408	
	Mo1-O5	1.901	1.016348413	Mo2-O12	1.896	1.03017607	
	Mo1-O1	2.046	0.686825051	Mo2-O9	2.09	0.609818081	
	Mo1-O4	2.151	0.517130789	Mo2-O11	2.151	0.517130789	
	Mo1-O2	2.256	0.389362986	Mo2-O8	2.222	0.426837734	
	BVS of Mo1		5.974659518		BVS of Mo2		5.972532448
	Te1-O4	1.889	1.268503473	Te2-O2	1.881	1.296229233	
	Te1-O5	1.917	1.176050937	Te2-O1	1.898	1.238020228	
	Te1-O3	1.953	1.067014823	Te2-O3	1.93	1.135447705	
	Te1-O2	2.381	0.33558101	Te2-O1	2.571	0.20080813	
	Te1-O4	2.466	0.266702461	Te2-O13	2.754	0.122456428	
				Te2-O6	2.79	0.111103031	
	BVS of Te1		4.113852704		BVS of Te2		4.104064755
	Te3-O11	1.89	1.265079714	Te4-O8	1.891	1.261665196	
	Te3-O12	1.929	1.138520633	Te4-O9	1.908	1.205008338	
	Te3-O10	1.948	1.08153181	Te4-O10	1.927	1.144691462	
	Te3-O8	2.354	0.360984983	Te4-O8	2.561	0.206309383	
Te3-O11	2.44	0.28611789	Te4-O11	2.713	0.136806305		
BVS of Te3		4.13223503		BVS of Te4		3.954480683	

(a)



(b)



Fig. S1. Digital images of $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ (a) and $\beta\text{-MoTe}_2\text{O}_7$ (b).

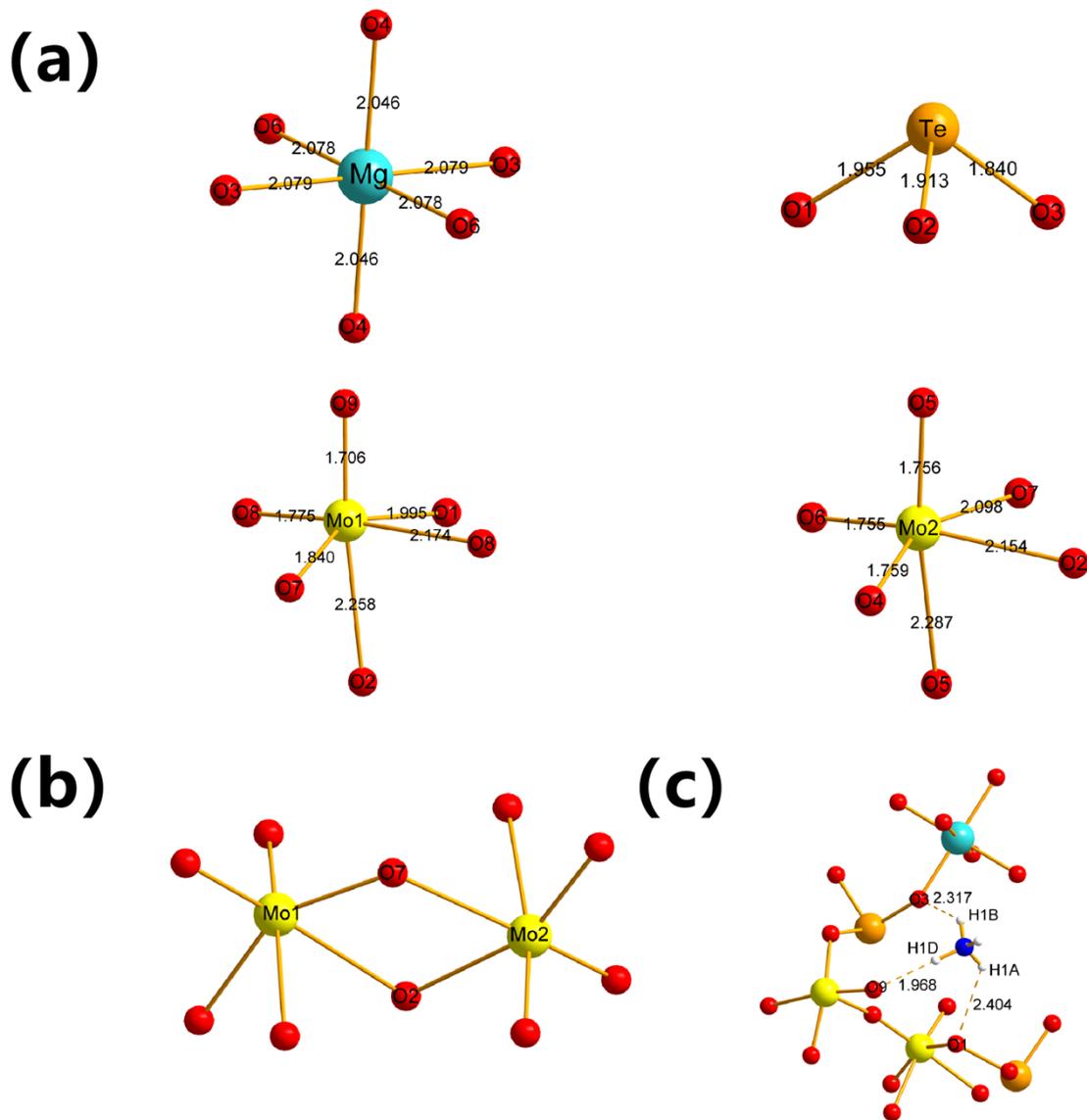


Fig. S2. (a) The coordinated environments of Mg, Te, Mo1 and Mo2 atoms in $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$. (b) Mo_2O_{10} edge-sharing dimers. (c) The coordinated environments of H atoms in $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$.

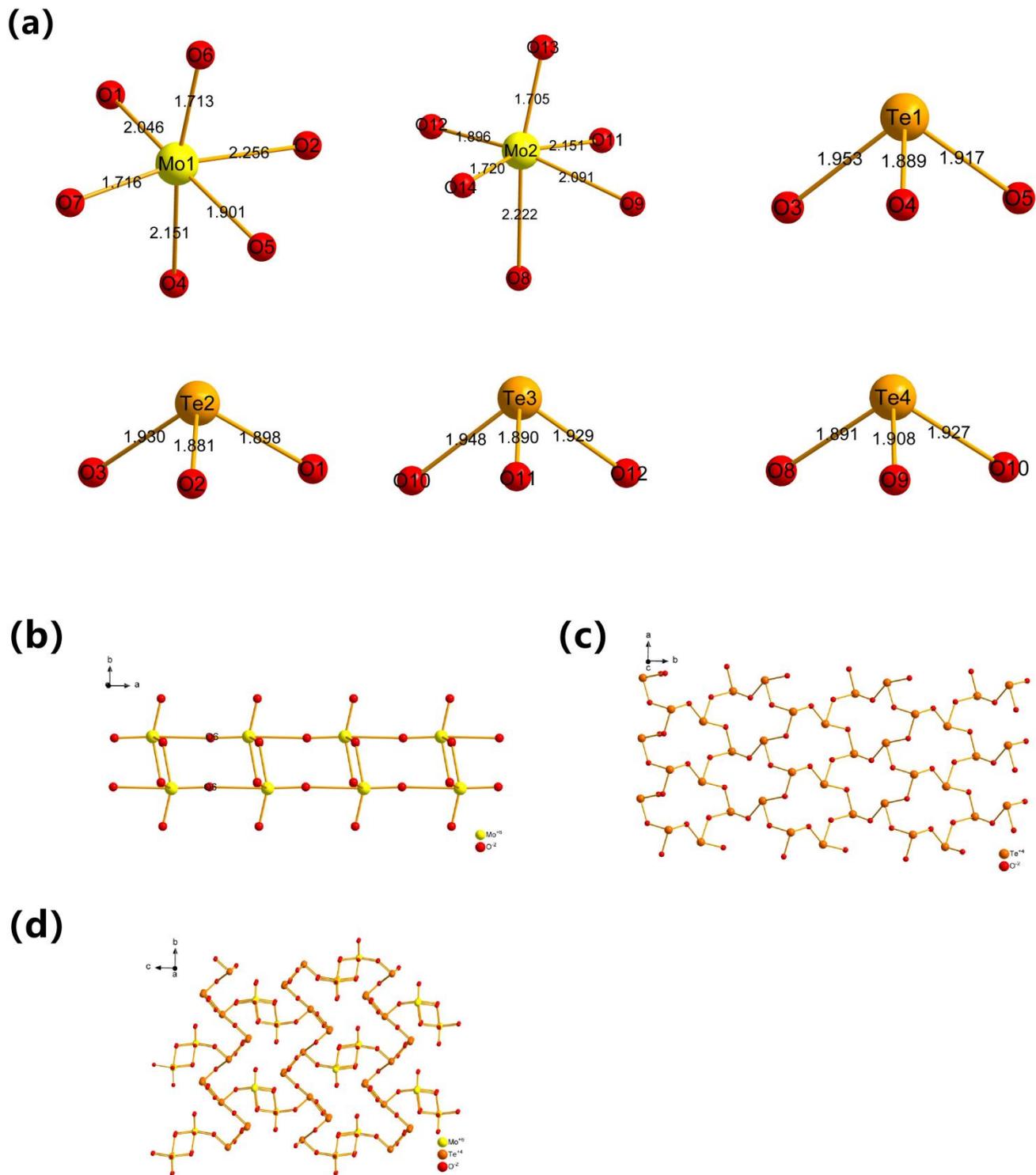
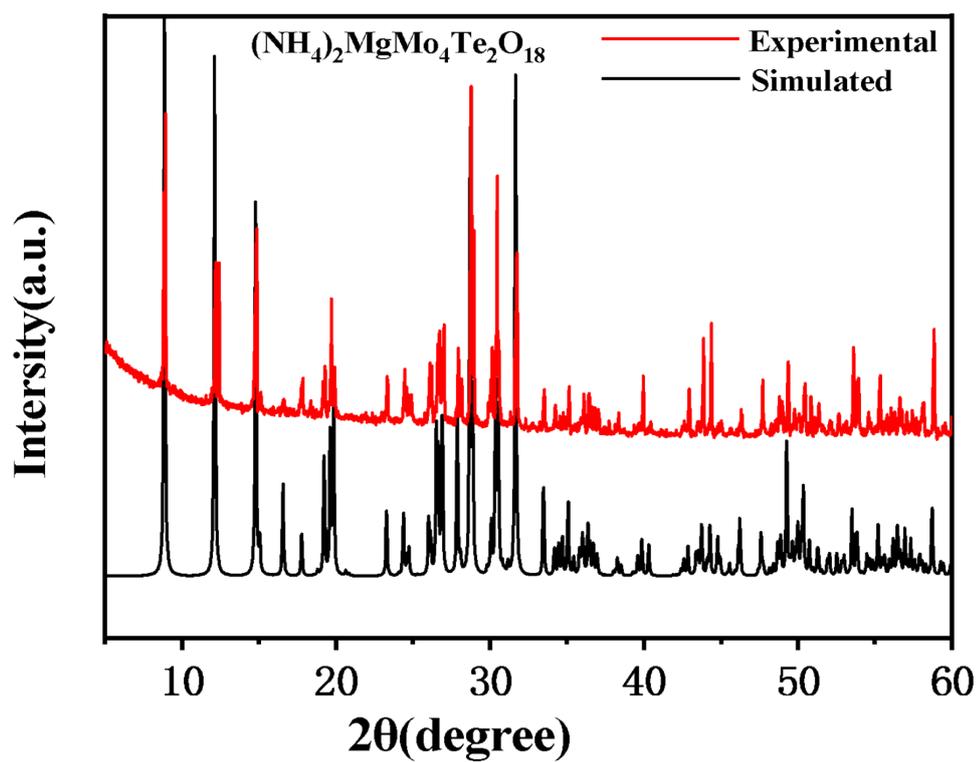


Fig. S3. (a) The coordinated environments of Mo1, Mo2, Te1, Te2, Te3 and Te4 atoms in β - MoTe_2O_7 . (b) a ladder-like one-dimensional $[\text{Mo-O}]_\infty$ chain in α - MoTe_2O_7 . (c) The TeO_3 trigonal pyramids in α - MoTe_2O_7 polymerize into a zigzag chain along b-axis. (d) 3D framework of α - MoTe_2O_7

(a)



(b)

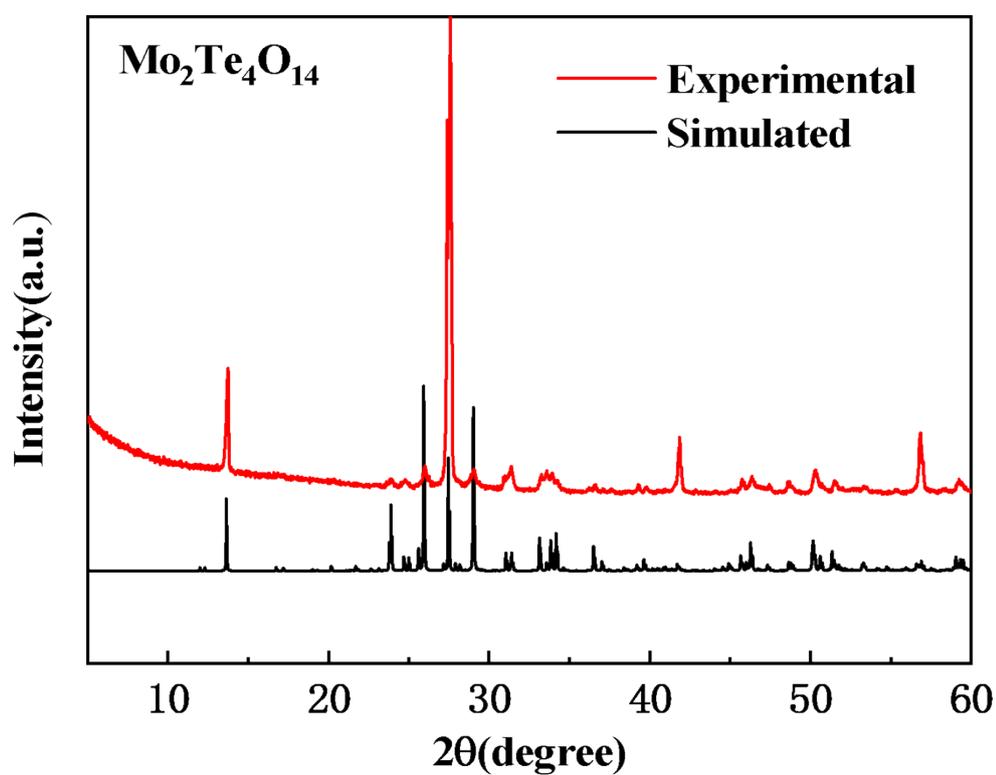
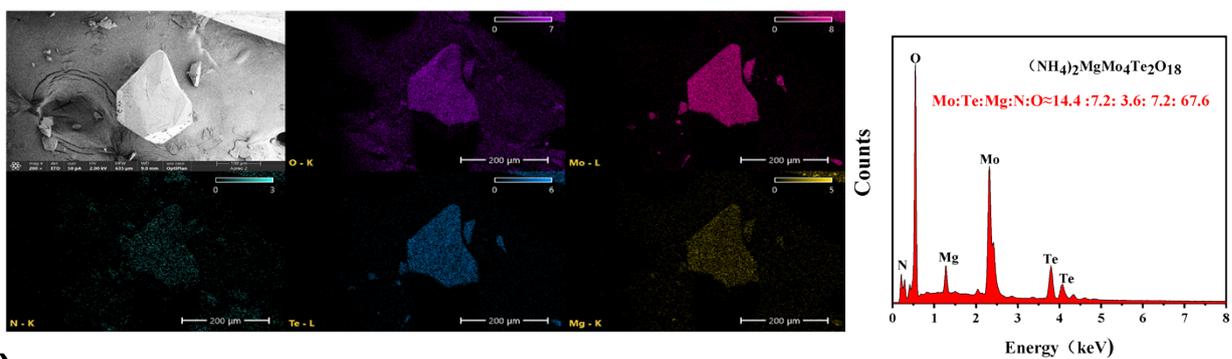


Fig. S4. Experimental and simulated XRD patterns of $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ (a) and $\beta\text{-MoTe}_2\text{O}_7$ (b).

(a)



(b)

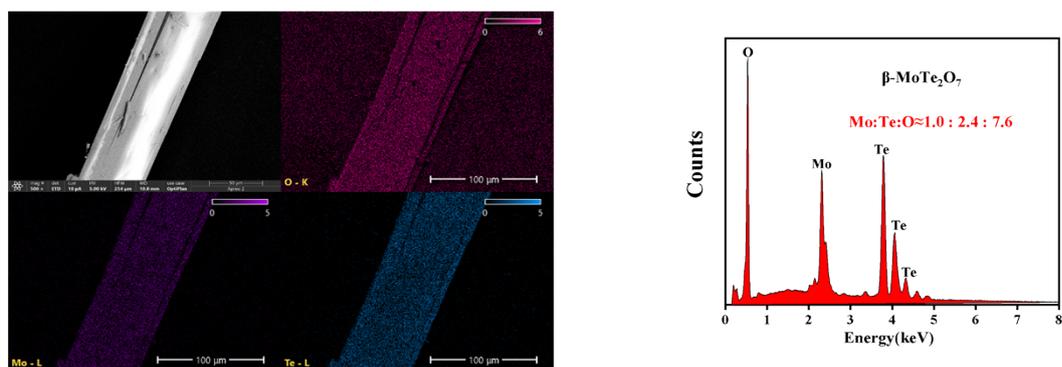
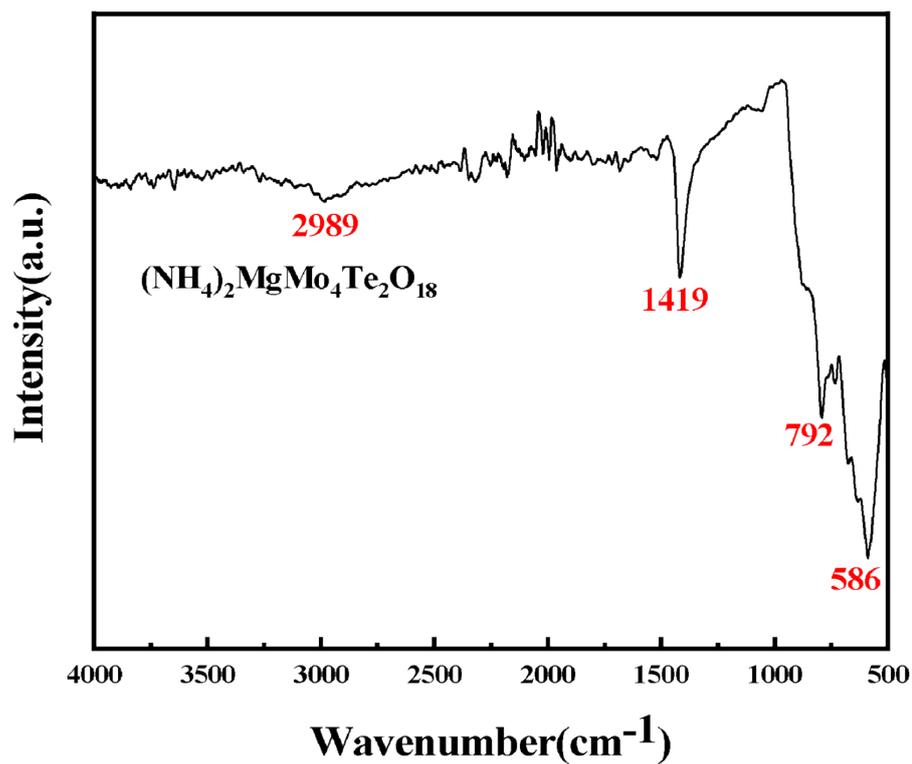


Fig. S5. SEM image and Elemental mapping and EDS spectrum of $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ (a) and $\beta\text{-MoTe}_2\text{O}_7$ (b).

(a)



(b)

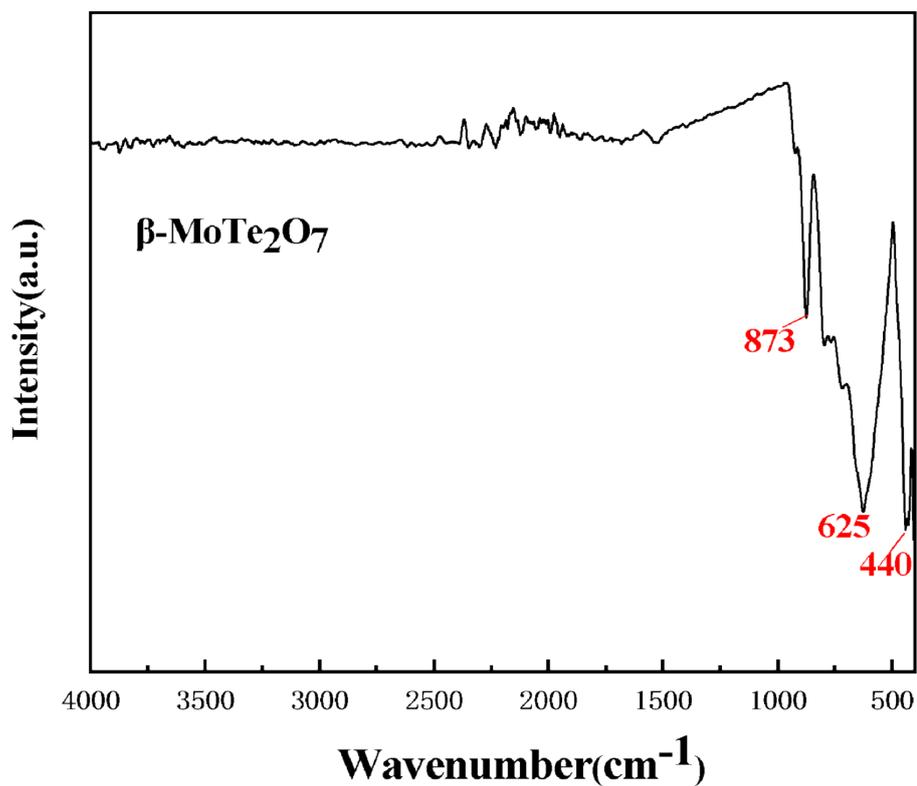


Fig. S6. Infrared absorption spectra of $(\text{NH}_4)_2\text{MgMo}_4\text{Te}_2\text{O}_{18}$ (a) and $\beta\text{-MoTe}_2\text{O}_7$ (b).

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I. Brown, I. D. J. P.; Minerals, C. o., Recent developments in the bond valence model of inorganic bonding. *Physics and Chemistry of Minerals* **1987**, *15* (1), 30-34.