

## Explorations of New Phases in the Ga<sup>III</sup>/In<sup>III</sup>-Mo<sup>VI</sup>-Se<sup>IV</sup>/Te<sup>IV</sup>-O Systems

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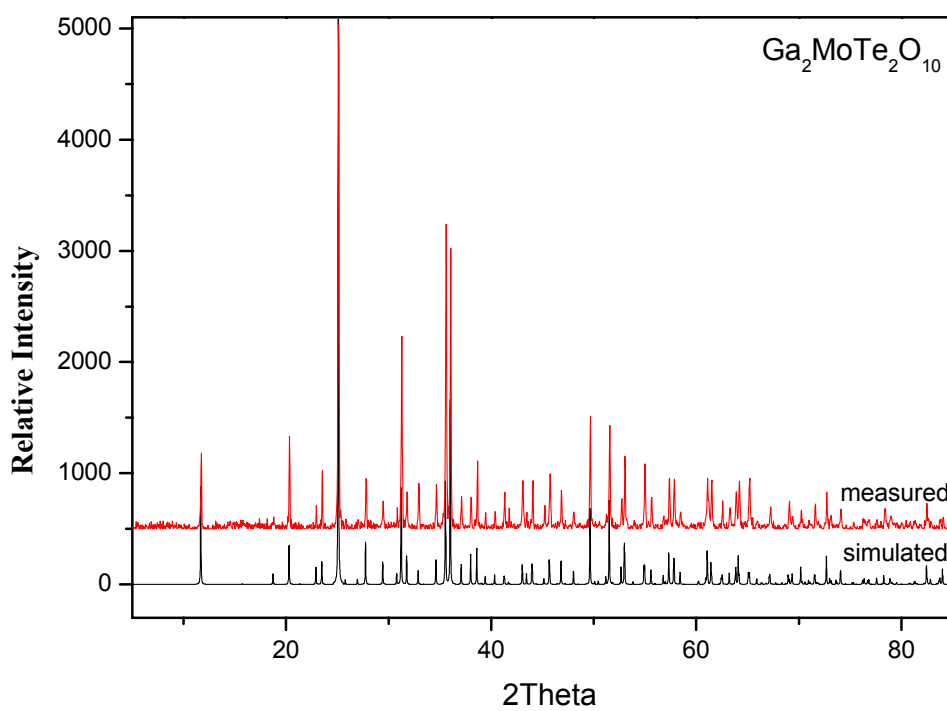
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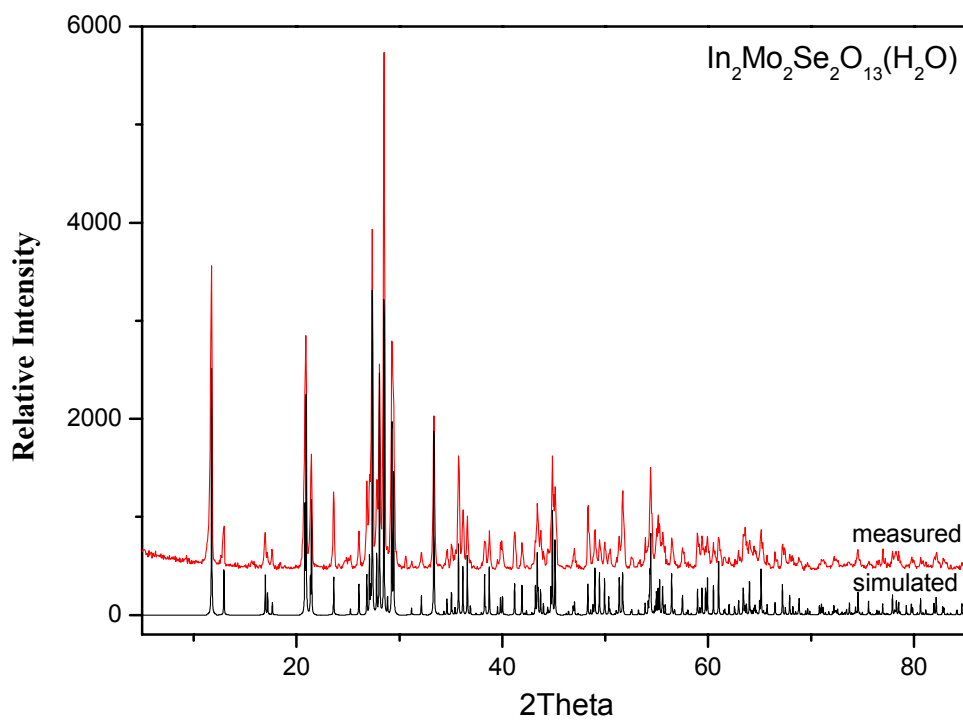
Table S1. The calculated bond orders of the compounds.

For Ga <sub>2</sub> MoSe <sub>2</sub> O <sub>10</sub>					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
Mo-O	1.69352	0.83	Mo-O	1.88337	0.49
Mo-O	1.96313	0.39	Mo-O	2.51539	0.10
Se-O	1.68245	0.41	Se-O	1.69313	0.34
Se-O	1.75660	0.40	Se-O	1.76398	0.38
Ga-O	1.92960	0.38	Ga-O	1.93502	0.35
Ga-O	1.97502	0.31	Ga-O	1.99222	0.29
Ga-O	1.99909	0.29	Ga-O	2.00771	0.27
For Ga <sub>2</sub> MoTe <sub>2</sub> O <sub>10</sub>					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
Mo-O	1.71744	0.81	Mo-O	1.84750	0.53
Mo-O	1.98267	0.39	Mo-O	2.37248	0.17
Te-O	1.86684	0.36	Te-O	1.88495	0.26
Te-O	1.88680	0.46	Te-O	1.92252	0.38
Ga-O	1.93246	0.41	Ga-O	1.93836	0.37
Ga-O	1.93991	0.35	Ga-O	1.98316	0.32
Ga-O	2.03986	0.26	Ga-O	2.05373	0.23
For In <sub>2</sub> Mo <sub>2</sub> Se <sub>2</sub> O <sub>13</sub> (H <sub>2</sub> O)					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
Mo-O	1.69069	0.81	Mo-O	1.72480	0.65
Mo-O	1.86255	0.49	Mo-O	1.90791	0.44
Mo-O	2.34809	0.18	Mo-O	2.48674	0.06
Se-O	1.68310	0.45	Se-O	1.68601	0.35
Se-O	1.72557	0.29	H-O	0.85047	0.64
In-O	2.08108	0.36	In-O	2.13407	0.35

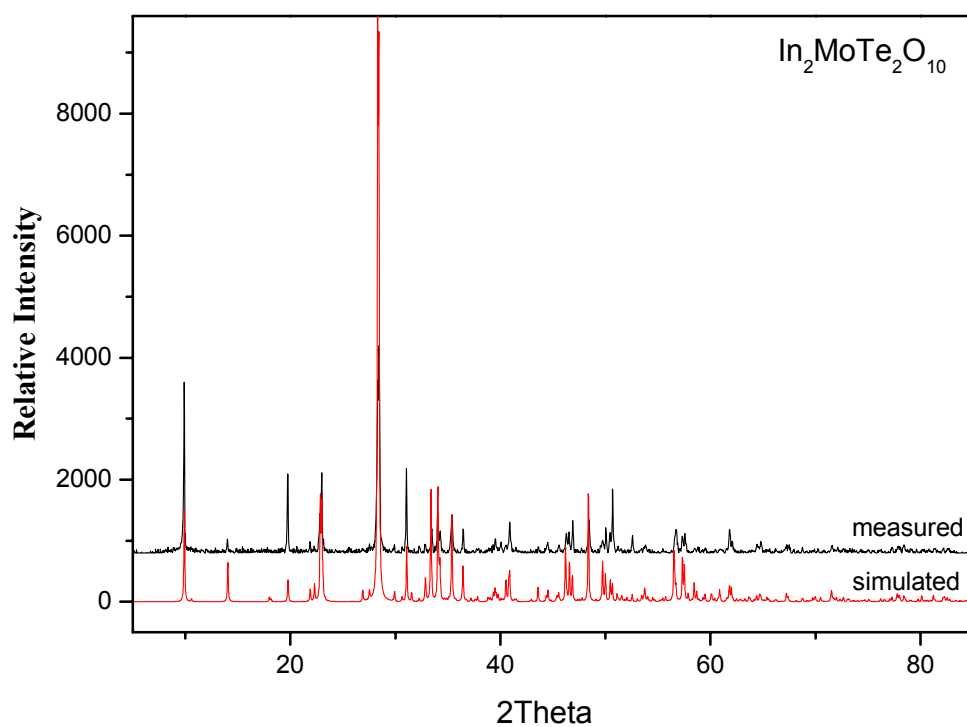
In-O	2.13890	0.24	In-O	2.14715	0.27
In-O	2.18705	0.22	In-O	2.20779	0.18
For In <sub>2</sub> MoTe <sub>2</sub> O <sub>10</sub>					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
Mo-O	1.71623	0.77	Mo-O	1.72597	0.76
Mo-O	1.82644	0.60	Mo-O	1.86957	0.58
Te-O	1.89831	0.35	Te-O	1.91024	0.37
Te-O	1.94459	0.26	Te-O	1.94603	0.30
Te-O	1.94730	0.30	Te-O	1.97384	0.25
In-O	2.09602	0.38	In-O	2.11609	0.36
In-O	2.11984	0.34	In-O	2.14641	0.31
In-O	2.17663	0.30	In-O	2.18178	0.30
In-O	2.19924	0.29	In-O	2.20406	0.24
In-O	2.21005	0.27	In-O	2.28709	0.21
In-O	2.34267	0.16	In-O	2.36115	0.20



(a)

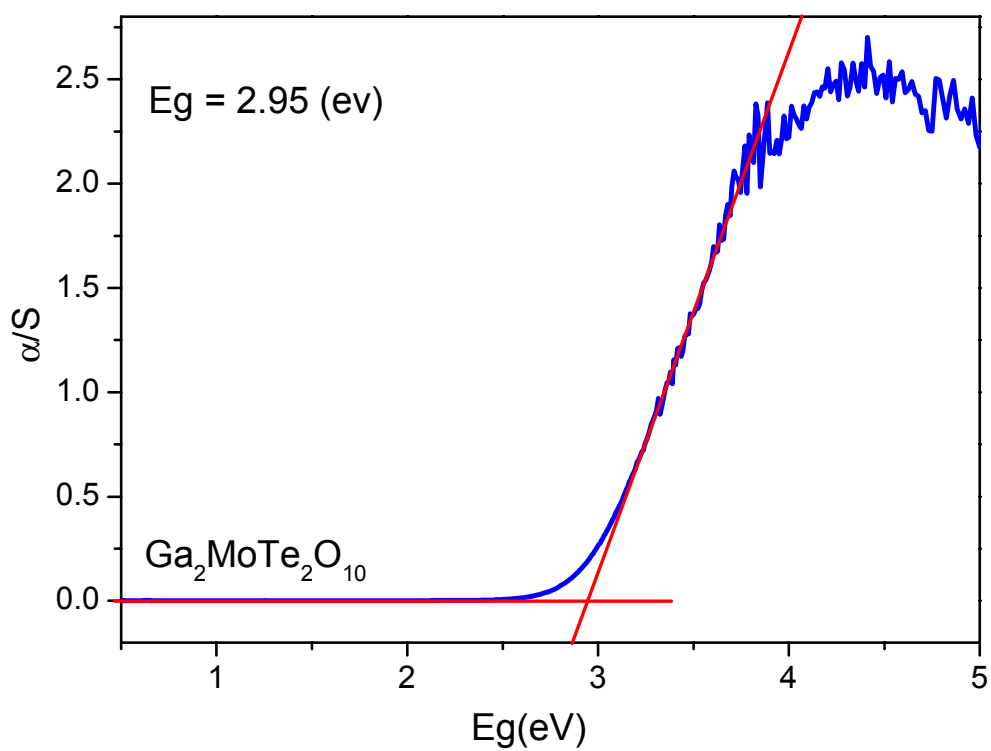


(b)

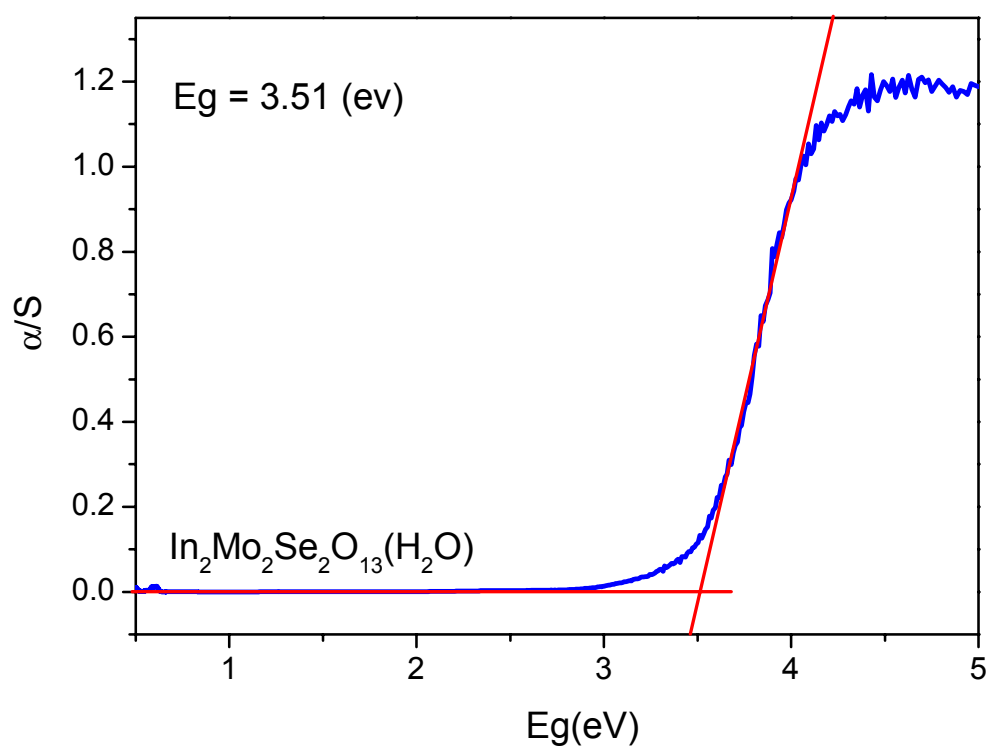


(c)

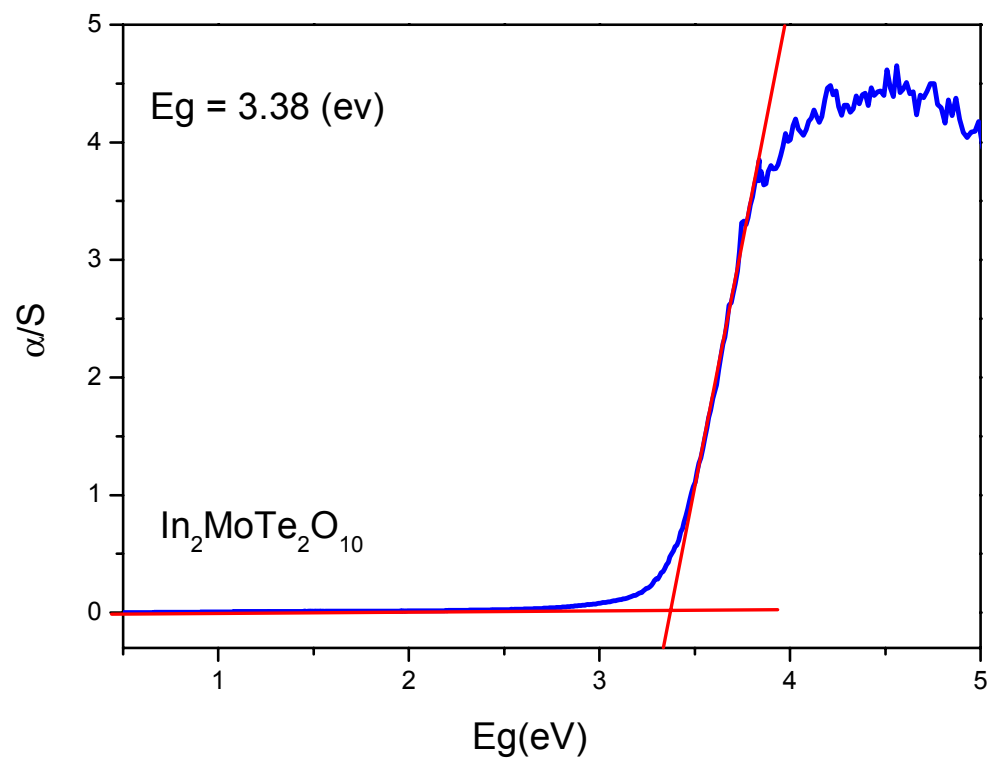
Figure S1. Simulated and measured XRD powder patterns for  $\text{Ga}_2\text{MoTe}_2\text{O}_{10}$  (a),  $\text{In}_2\text{Mo}_2\text{Se}_2\text{O}_{13}(\text{H}_2\text{O})$  (b) and  $\text{In}_2\text{MoTe}_2\text{O}_{10}$  (c).



(a)

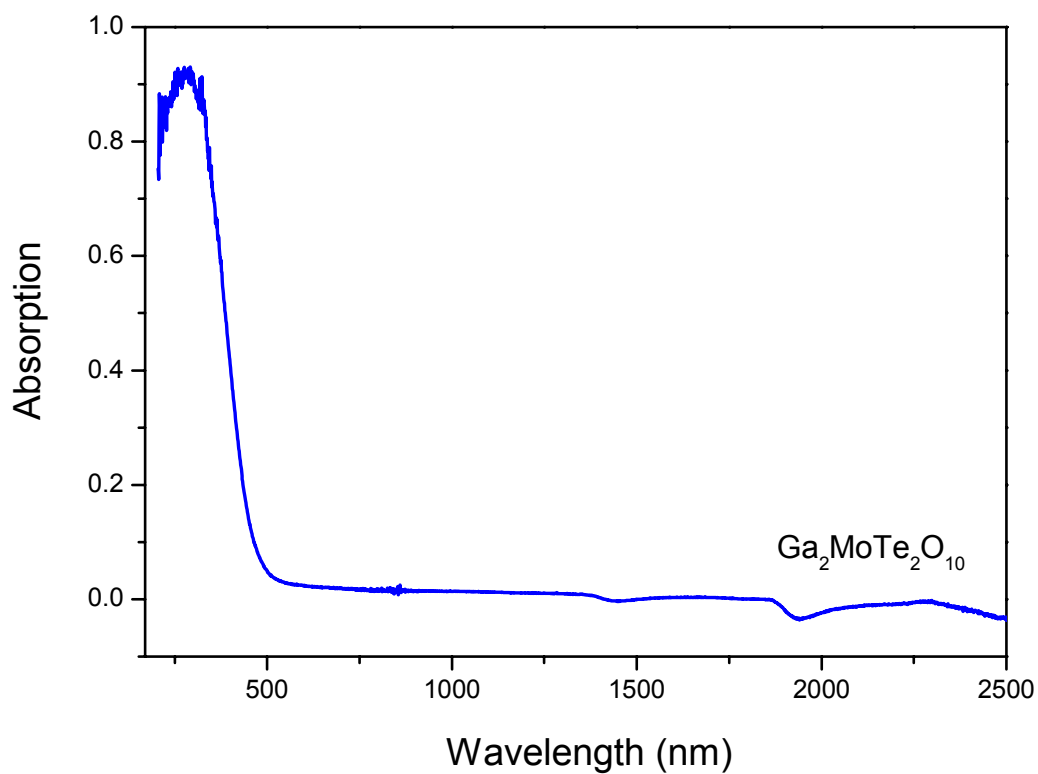


(b)

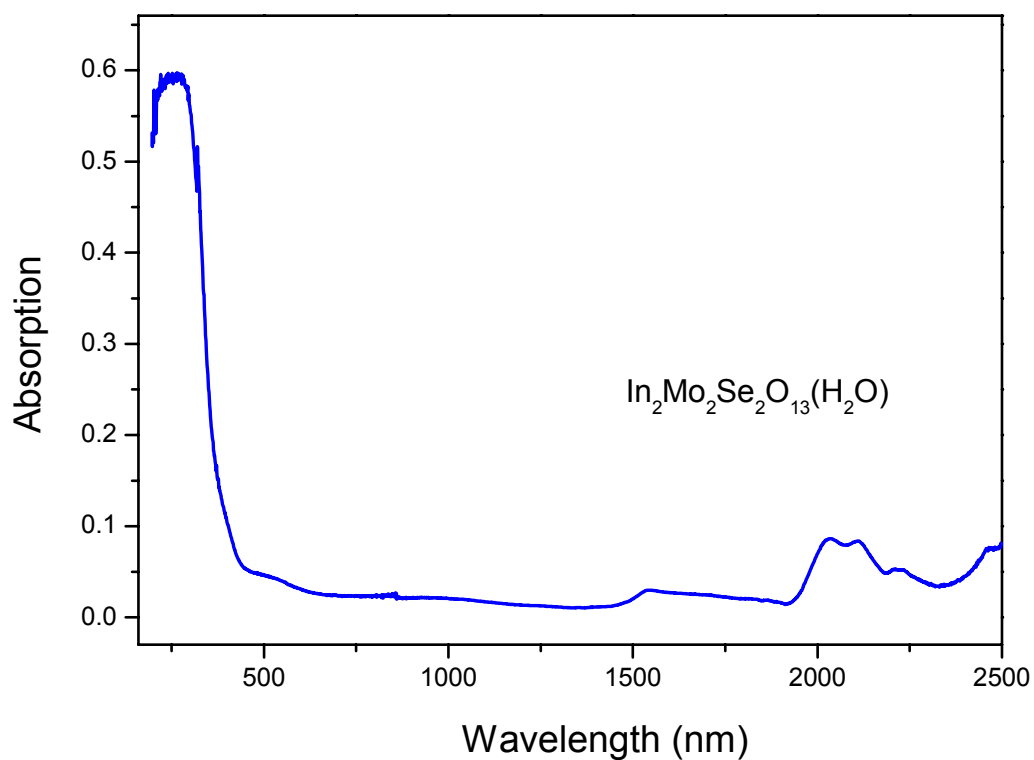


(c)

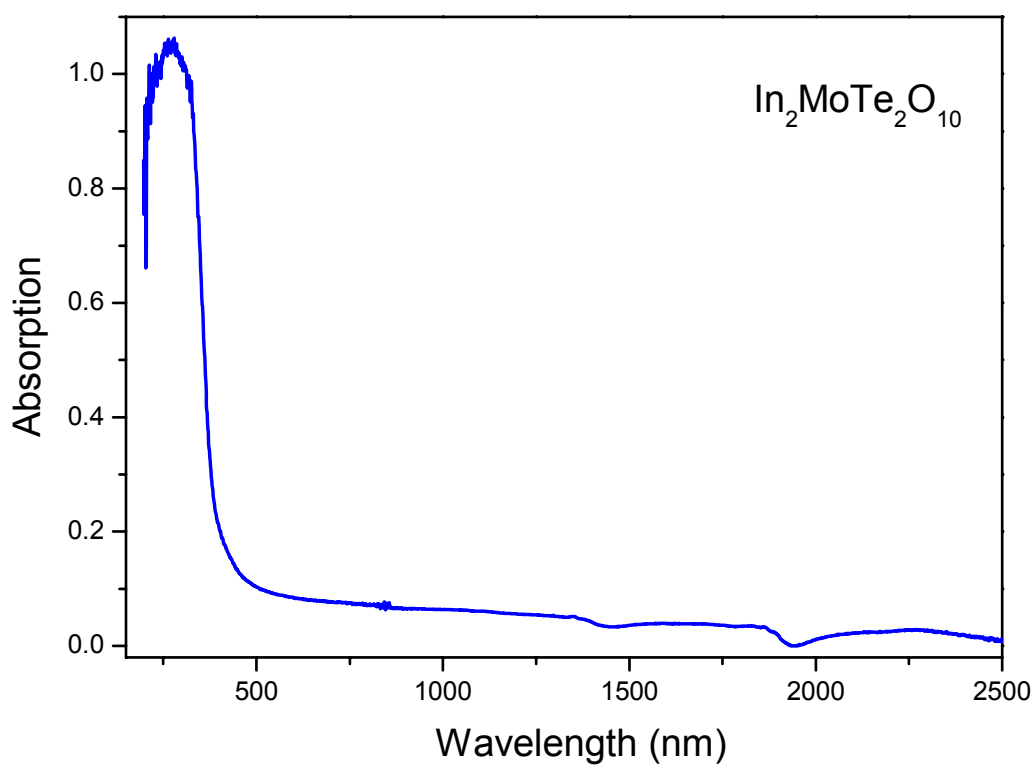
Figure S2. Optical diffuse reflectance spectra for  $\text{Ga}_2\text{MoTe}_2\text{O}_{10}$  (a),  $\text{In}_2\text{Mo}_2\text{Se}_2\text{O}_{13}(\text{H}_2\text{O})$  (b) and  $\text{In}_2\text{MoTe}_2\text{O}_{10}$  (c).



(a)

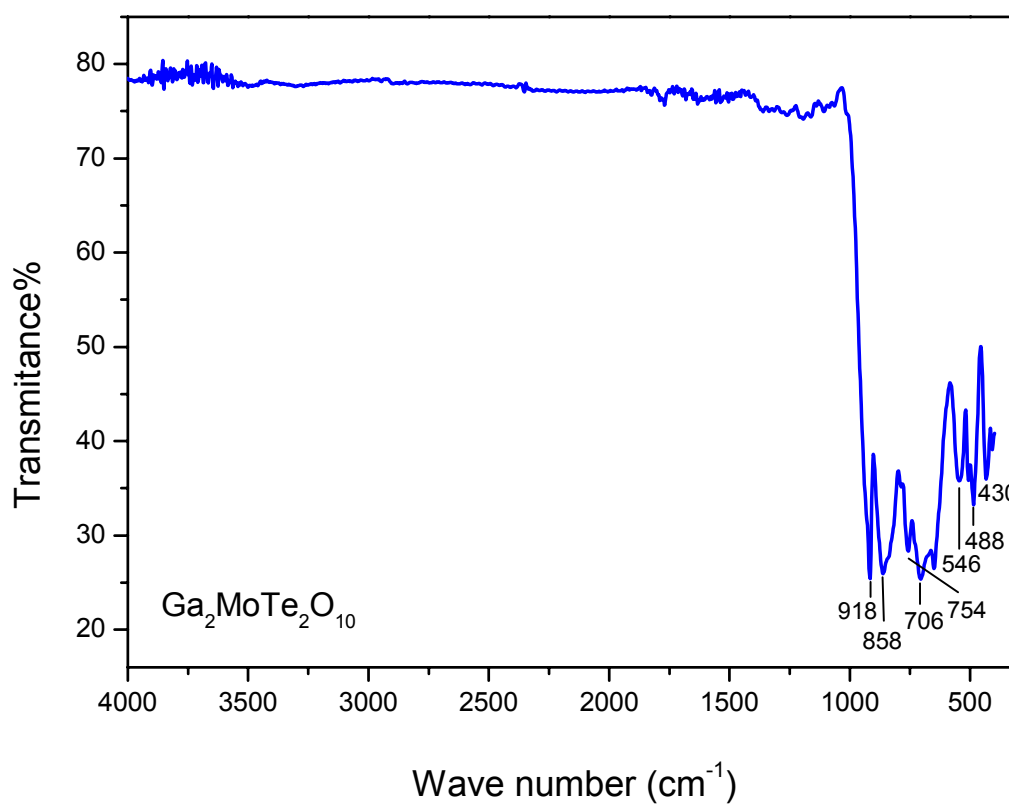


(b)

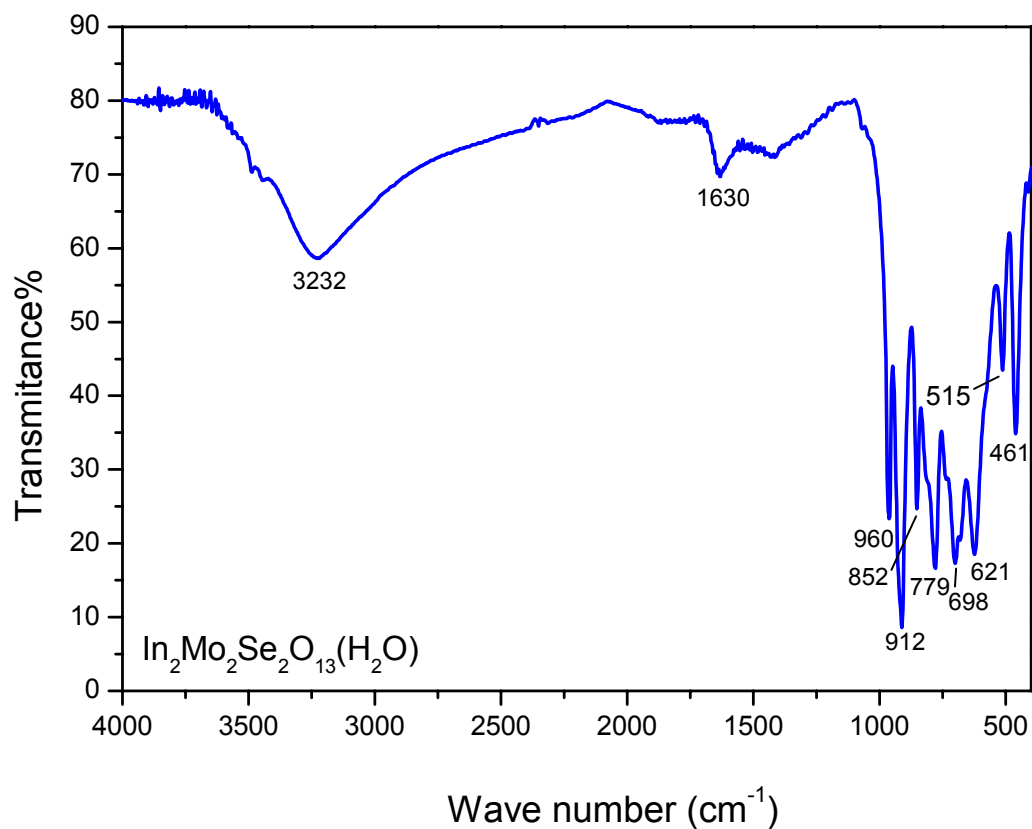


(c)

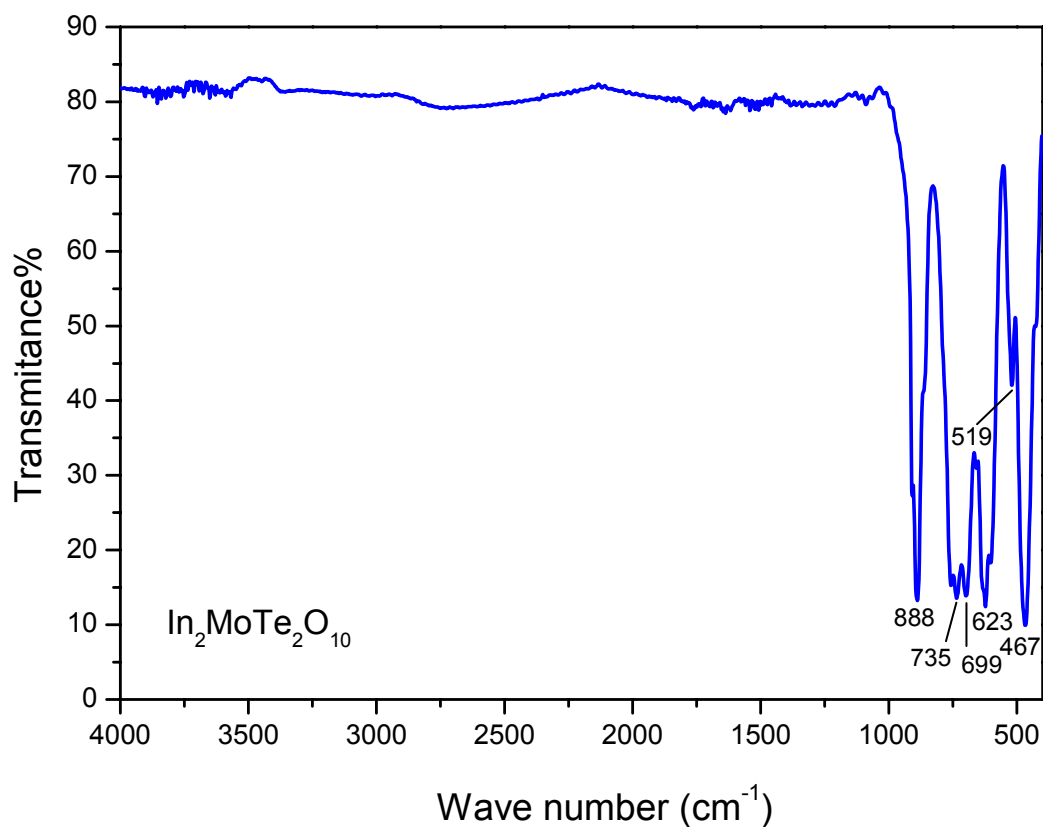
Figure S3. UV absorption spectra of  $\text{Ga}_2\text{MoTe}_2\text{O}_{10}$  (a),  $\text{In}_2\text{Mo}_2\text{Se}_2\text{O}_{13}(\text{H}_2\text{O})$  (b) and  $\text{In}_2\text{MoTe}_2\text{O}_{10}$  (c).



(a)



(b)





(c)

Figure S4. IR spectra of  $\text{Ga}_2\text{MoTe}_2\text{O}_{10}$  (a),  $\text{In}_2\text{Mo}_2\text{Se}_2\text{O}_{13}(\text{H}_2\text{O})$  (b) and  $\text{In}_2\text{MoTe}_2\text{O}_{10}$  (c).

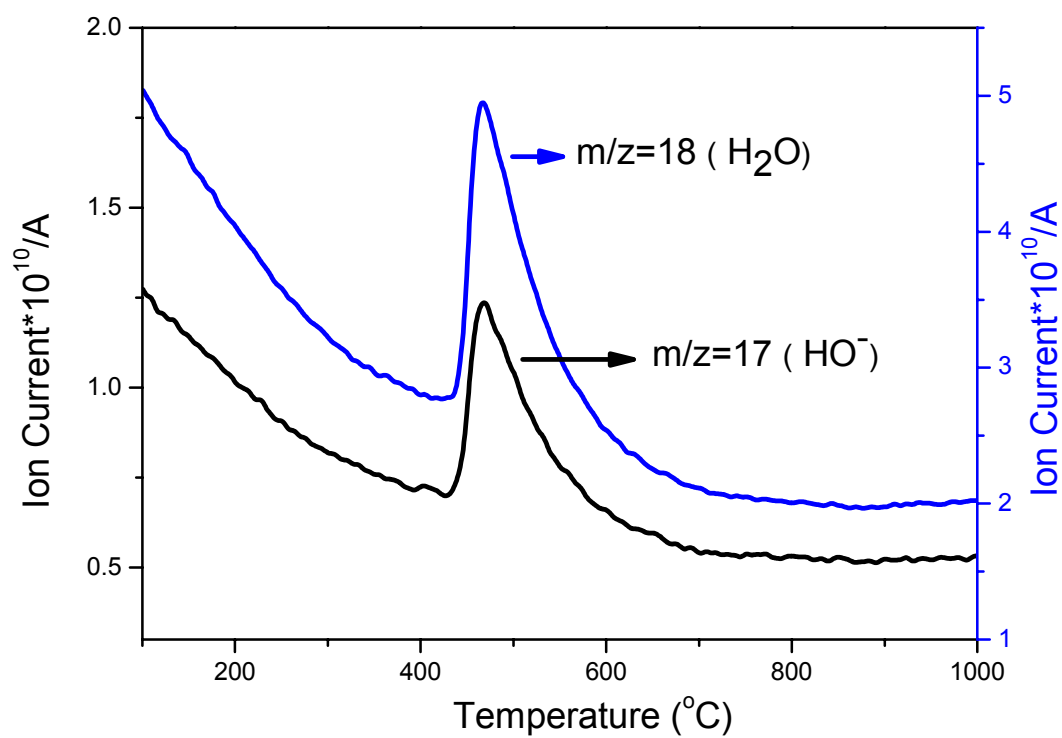


Figure S5. MS curves of  $\text{In}_2\text{Mo}_2\text{Se}_2\text{O}_{13}(\text{H}_2\text{O})$ .