

Supporting information for

**LaMTeO₆ (*M* = Ga³⁺ and Mn³⁺): the critical role of electronic
configuration and cation ordering in crystal structures**

Shunjie Tang,^a Yuxuan Qi,^b Pengfei Jiang,^{*a} and Tao Yang^{*a}

^a College of Chemistry and Chemical Engineering, Chongqing University, Chongqing
401331, China.

^b Chongqing Academy of Metrology & Quality Inspection, Chongqing 401121, China.

Corresponding authors: pengfeijiang@cqu.edu.cn; taoyang@cqu.edu.cn.

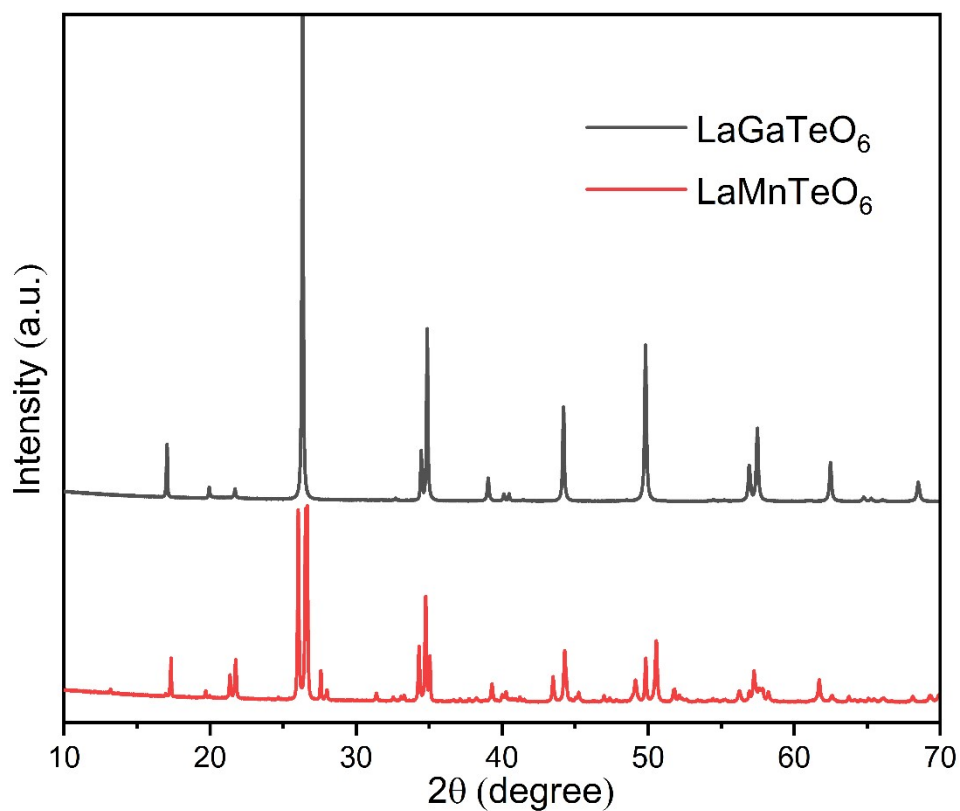


Fig. S1 High-resolution XRPD patterns for LaMTeO_6 with $M = \text{Ga}^{3+}$ and Mn^{3+} .

Table S1. Selected interatomic bond distances for trigonal LaGaTeO_6 .

| bond | length (Å) |
|-----------|------------|
| La-O1 × 6 | 2.413(2) |
| Ga-O1 × 6 | 1.980(2) |
| Te-O1 × 6 | 1.972(2) |

Table S2. Selected interatomic bond distances for monoclinic LaMnTeO₆.

| bond | length (Å) |
|--------|------------|
| La-O1 | 2.494(8) |
| La-O2 | 2.489(8) |
| La-O3 | 2.373(8) |
| La-O4 | 2.41(1) |
| La-O5 | 2.386(8) |
| La-O6 | 2.53(1) |
| <La-O> | 2.446 |
| Mn-O1 | 2.017(8) |
| Mn-O2 | 1.868(8) |
| Mn-O3 | 1.909(9) |
| Mn-O4 | 2.10(1) |
| Mn-O5 | 2.09(1) |
| Mn-O6 | 2.004(7) |
| <Mn-O> | 1.997 |
| Te-O1 | 1.940(7) |
| Te-O2 | 2.042(8) |
| Te-O3 | 2.044(9) |
| Te-O4 | 1.944(7) |
| Te-O5 | 1.94(1) |
| Te-O6 | 1.88(1) |
| <Te-O> | 1.964 |