Supporting Information (SI) for:

Cation Size Effect on the Formation of Centrosymmetric $AMo_2O_5(SeO_3)_2$ (A = Sr and Pb) and Noncentrosymmetric $BaMo_2O_5(SeO_3)_2$

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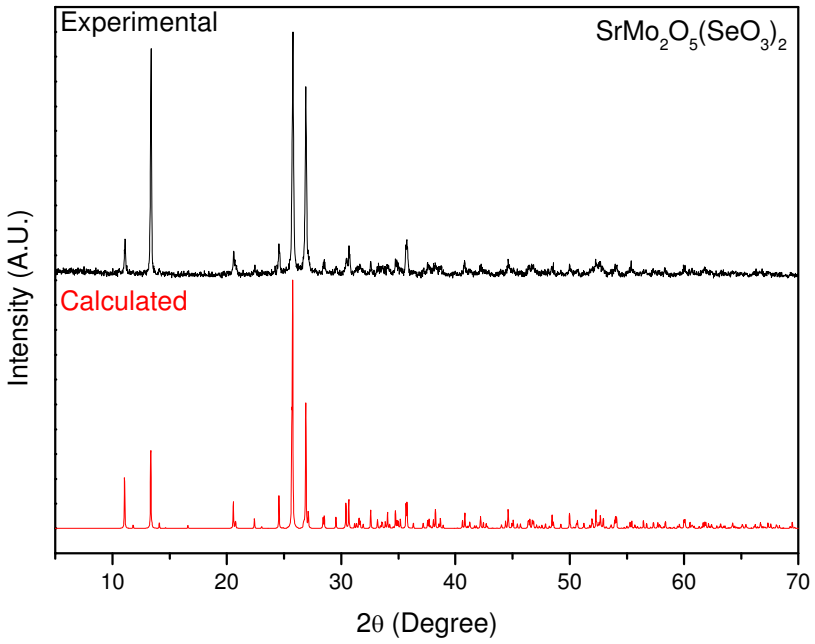
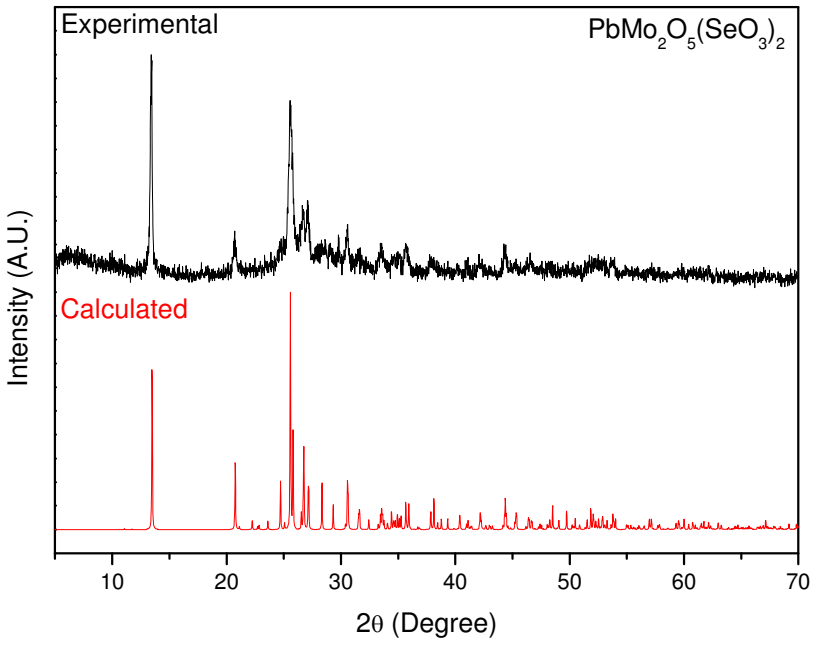
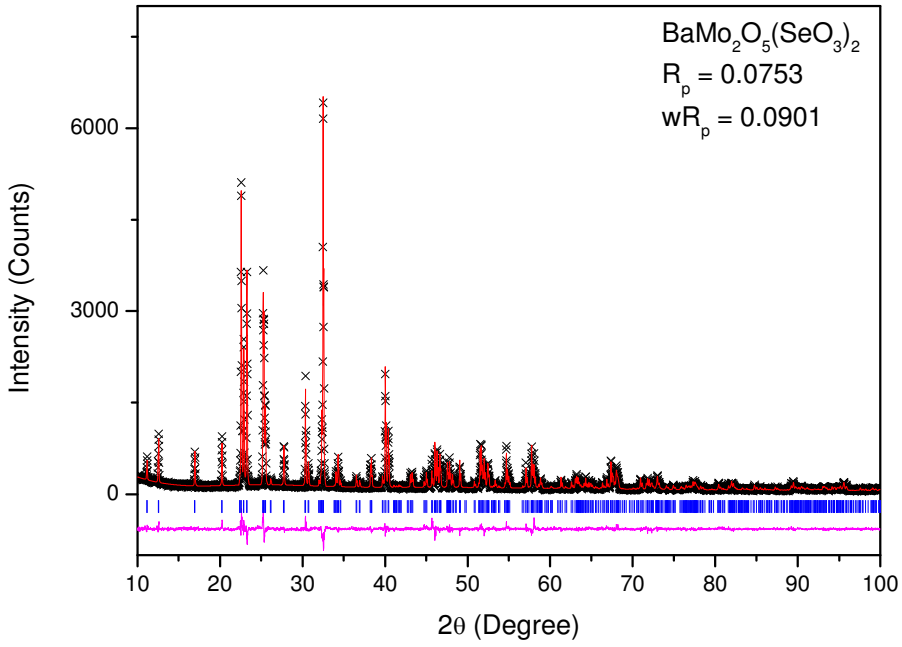
S1. Experimental and calculated powder X-ray diffraction patterns for $SrMo_2O_5(SeO_3)_2$



S2. Experimental and calculated powder X-ray diffraction patterns for $PbMo_2O_5(SeO_3)_2$

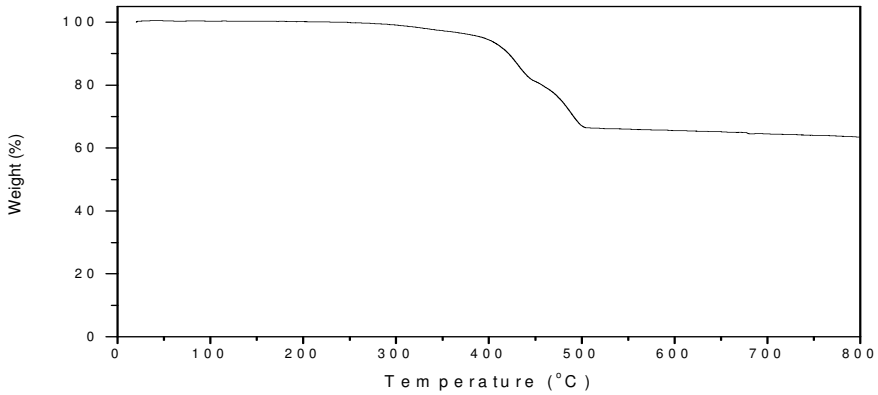


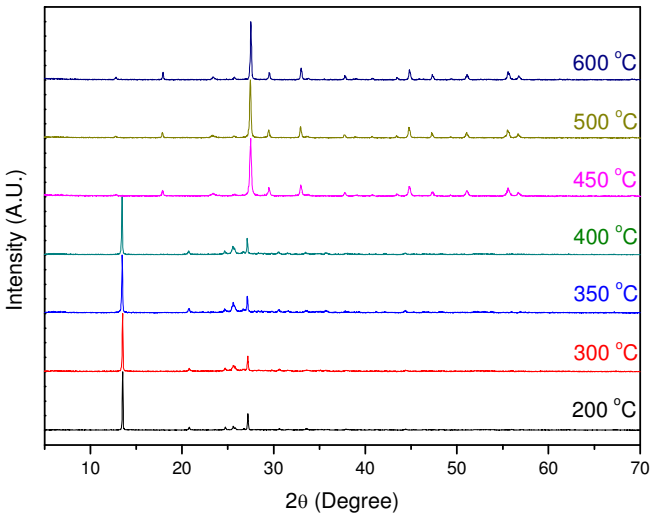
S3. Powder X-ray diffraction pattern matching plot for $BaMo_2O_5(SeO_3)_2$

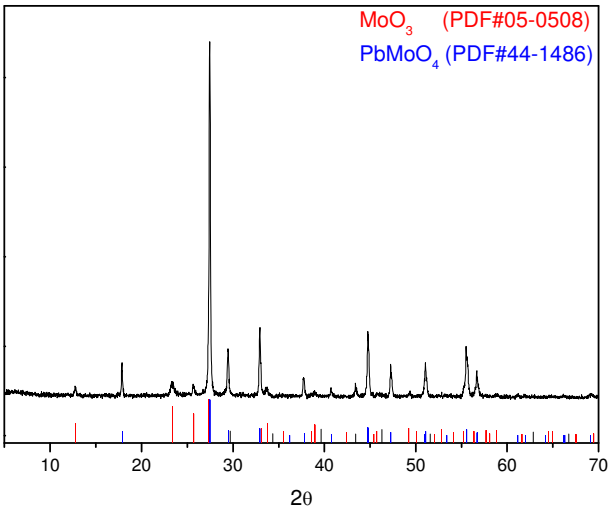


The calculated pattern (red solid line) is compared with observed data (×). The locations of reflections are indicated by the blue vertical bars. The difference between the observed and calculated profiles is shown at the bottom (magenta solid line).

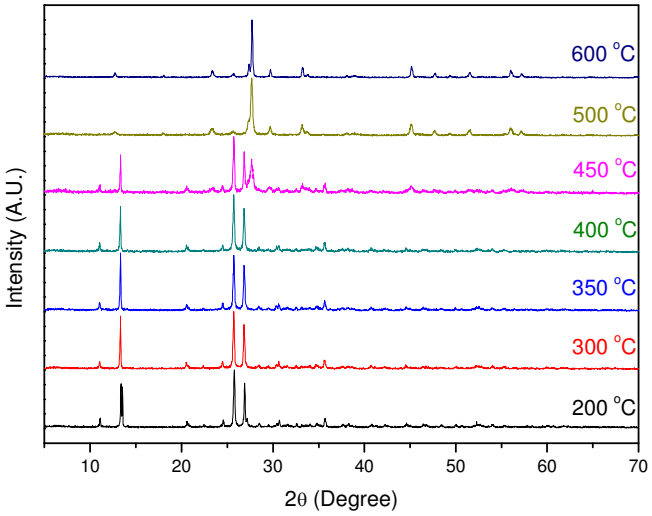
S4. Thermogravimetric analysis diagram, powder XRD patterns at different temperatures, and XRD pattern for calcined product for $PbMo_2O_5(SeO_3)_2$

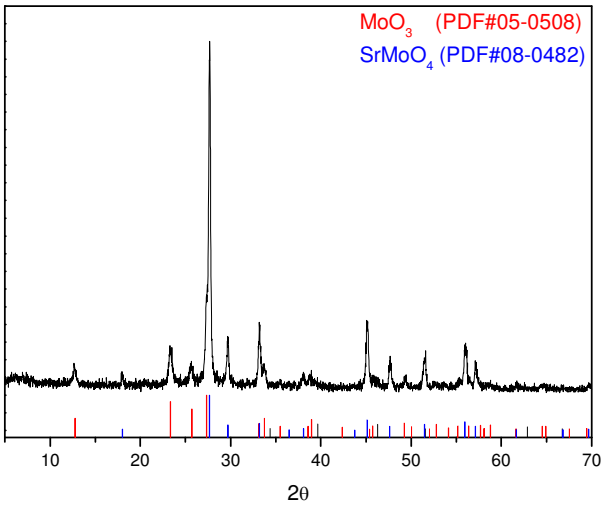




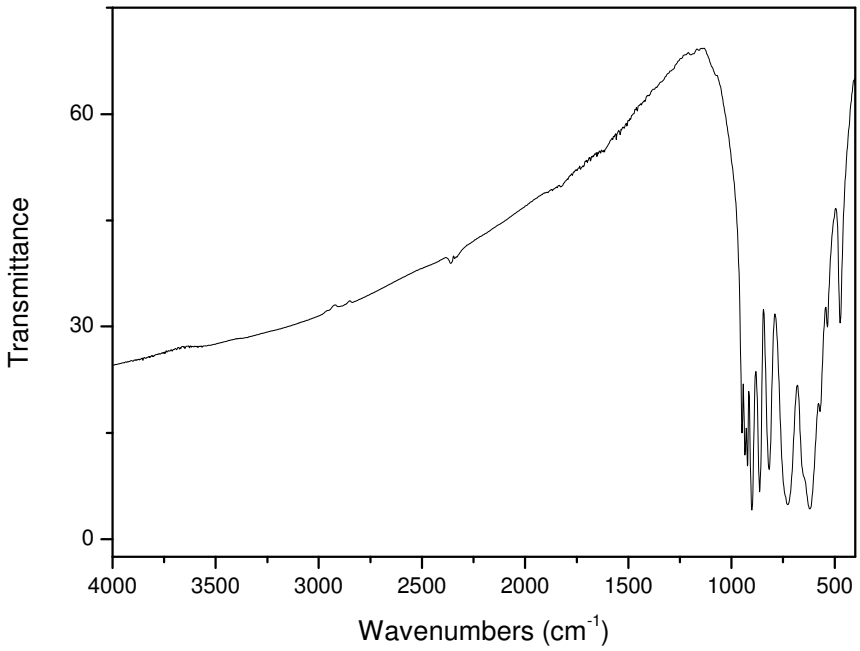


S5. Powder XRD patterns at different temperatures and XRD pattern for calcined product for $SrMo_2O_5(SeO_3)_2$





S6. IR spectrum for $SrMo_2O_5(SeO_3)_2$



S7. IR spectrum for $PbMo_2O_5(SeO_3)_2$