Electronic Supplementary Material (ESI) for Dalton Transactions
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Electronic Supplementary Information (ESI) for:

$PbMSeO_6$ (M = Mo and W): New quaternary mixed metal selenites with asymmetric cationic coordination environments

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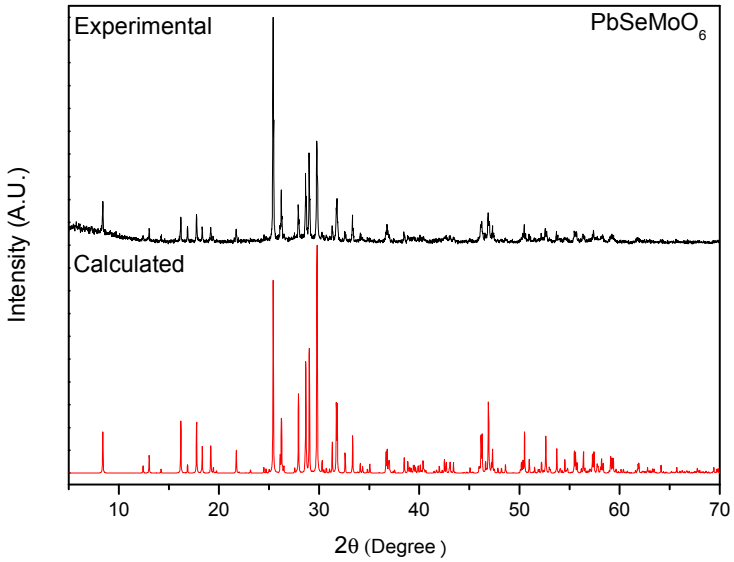
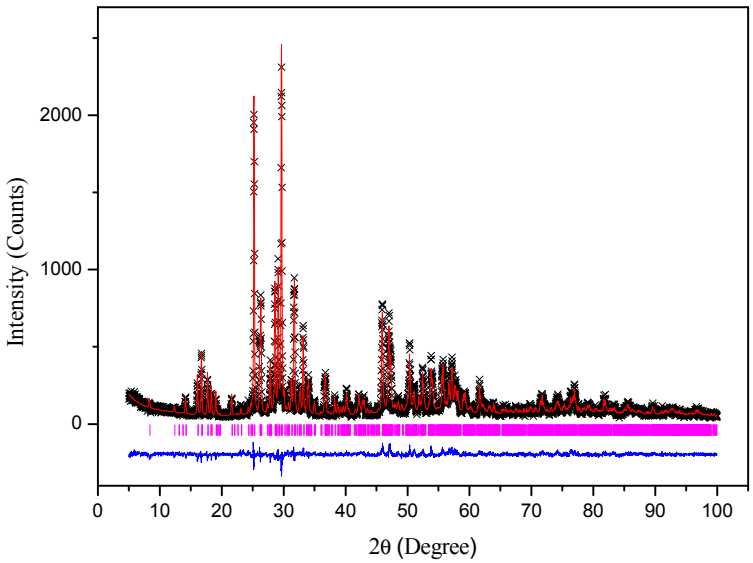
S1. Experimental and calculated powder X-ray diffraction patterns for $PbMoSeO_6$



S2. Final Rietveld plot of $PbWSeO_6$



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

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S3. Atomic positions and isotropic displacement parameters for $PbWSeO_6$

Atom	*x*	*y*	*z*	U_{iso} (Å^2)
Pb(1)	0.2451(9)	0.1375(11)	0.4936(5)	0.0238(2)
Pb(2)	0.3524(8)	0.2896(12)	0.1571(5)	0.0246(2)
W(1)	0.8396(9)	0.0473(11)	0.1985(6)	0.0224(2)
W(2)	0.8398(9)	0.5512(11)	0.2031(6)	0.0232(2)
Se(1)	0.712(2)	0.365(3)	0.4696(11)	0.0204(3)
Se(2)	0.3794(19)	0.810(3)	0.2145(12)	0.0223(3)
O(1)	0.828(9)	-0.044(10)	0.035(6)	0.02[a]
O(2)	1.115(9)	0.107(10)	0.244(6)	0.02[a]
O(3)	0.872(10)	-0.174(11)	0.273(5)	0.02[a]
O(4)	0.746(10)	0.296(14)	0.175(6)	0.02[a]
O(5)	0.807(10)	0.159(10)	0.404(5)	0.02[a]
O(6)	0.515(10)	0.974(10)	0.174(6)	0.02[a]
O(7)	0.822(9)	0.571(10)	0.042(5)	0.02[a]
O(8)	1.101(10)	0.494(9)	0.249(6)	0.02[a]
O(9)	0.794(10)	0.527(9)	0.404(5)	0.02[a]
O(10)	0.524(10)	0.607(9)	0.183(5)	0.02[a]
O(11)	0.471(9)	0.336(12)	0.399(6)	0.02[a]
O(12)	0.425(10)	0.857(11)	0.378(5)	0.02[a]

[a] Displacement parameters constrained to be equal.

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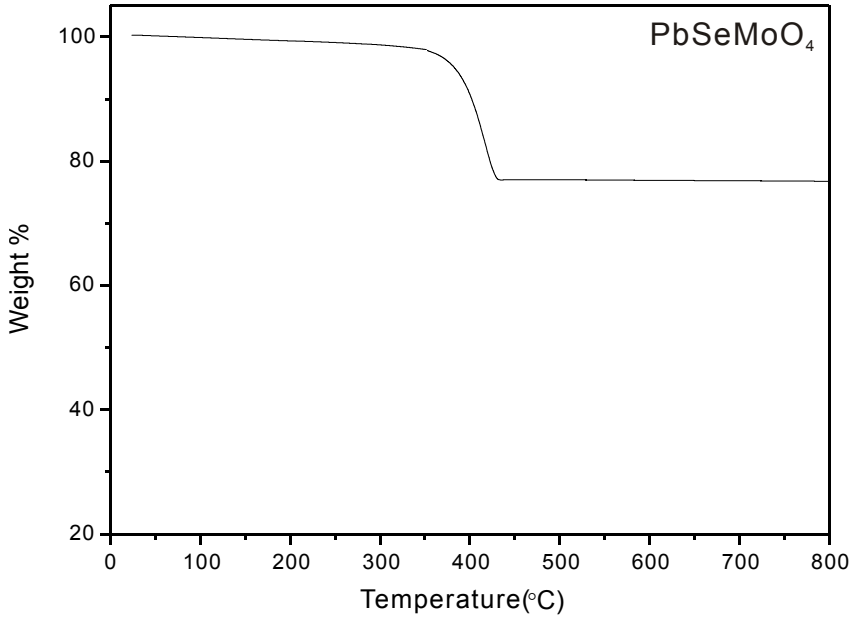
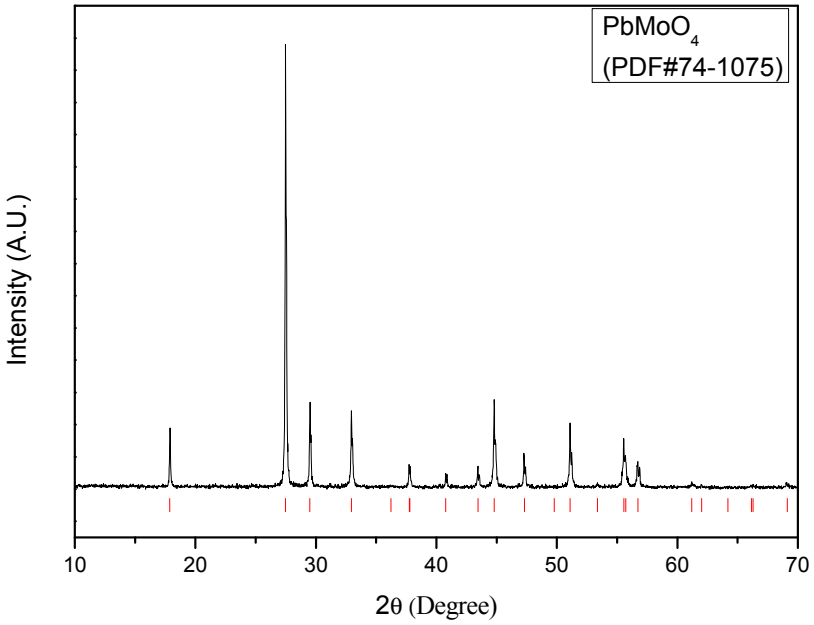
S4. Thermogravimetric analysis diagram for $PbMoSeO_6$ and XRD pattern for calcined product





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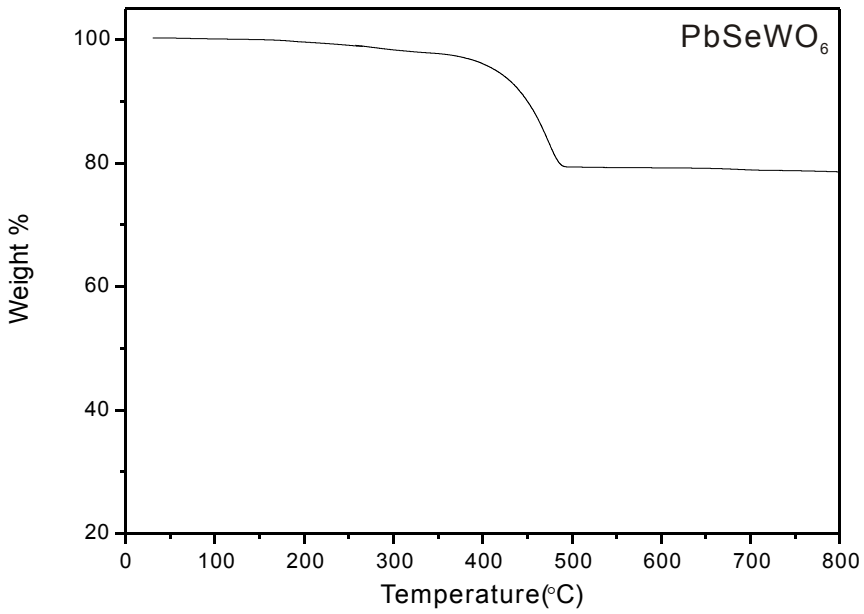
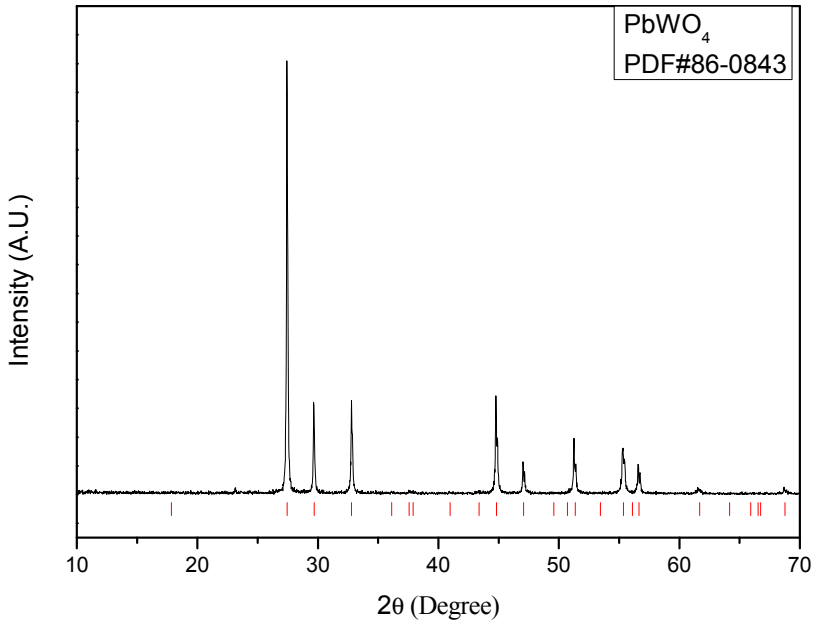
S5. Thermogravimetric analysis diagram for $PbWSeO_6$ and XRD pattern for calcined product





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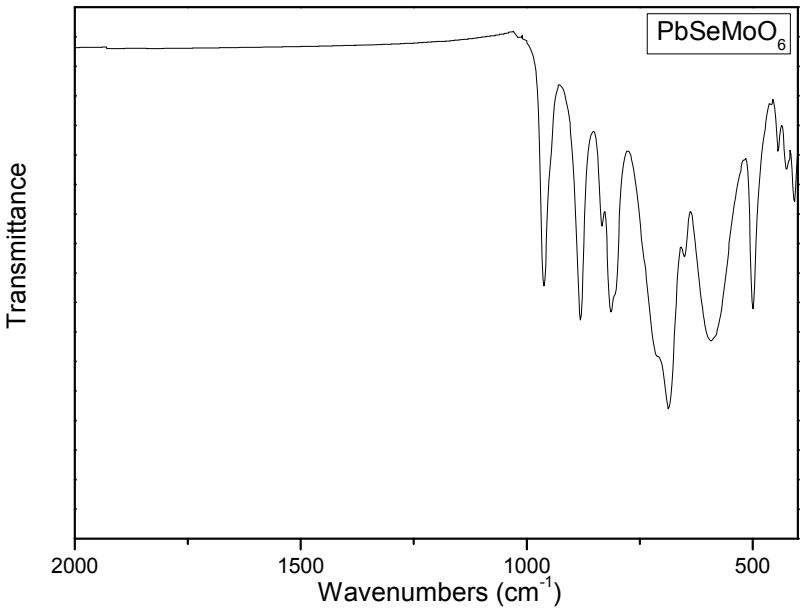
S6. IR spectrum for $PbMoSeO_6$



S7. IR spectrum for $PbWSeO_6$