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Supporting information for article:

Cs₃LiZn₂(WO₄)₄ and Rb₃Li₂Ga(MoO₄)₄: different filled derivatives of the cation-deficient Cs₆Zn₅(MoO₄)₈ structure

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S1. Computing details

For both compounds, data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); absorption correction: *SADABS* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL-97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *SHELXL-97*.

Table S1 Atomic coordinates and equivalent isotropic displacement parameters for $\text{Cs}_3\text{LiZn}_2(\text{WO}_4)_4$ and $\text{Rb}_3\text{Li}_2\text{Ga}(\text{MoO}_4)_4$

Atom	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	$U_{\text{eq}} (\text{\AA}^2)$
$\text{Cs}_3\text{LiZn}_2(\text{WO}_4)_4$				
Cs	0.8750	0	0.2500	0.0280(2)
W	0.40026(2)	0.40026(2)	0.40026(2)	0.0130(1)
(2Zn + Li)/3	0.3750	0	0.2500	0.0154(4)
O(1)	0.3185(4)	0.3185(4)	0.3185(4)	0.028(2)
O(2)	0.5312(4)	0.4081(4)	0.3375(4)	0.0238(10)
$\text{Rb}_3\text{Li}_2\text{Ga}(\text{MoO}_4)_4$				
Rb(1)	0	0	0	0.02889(13)
Rb(2)	0.36464(4)	0.2500	0.1250	0.02726(9)
Mo	0.10403(2)	0.14339(2)	0.27094(2)	0.01532(5)
Ga	0	0	0.5000	0.01470(10)
Li	-0.1246(6)	0.2500	0.1250	0.0178(13)
O(1)	0.1000(2)	0.0759(2)	0.4111(2)	0.0234(4)
O(2)	-0.0299(2)	0.1486(2)	0.2095(2)	0.0250(4)
O(3)	0.1896(2)	0.0633(2)	0.1856(2)	0.0270(5)
O(4)	0.1636(2)	0.2778(2)	0.2786(2)	0.0262(5)