

**Supporting Information for:**

**Preparation, crystal structure and luminescence properties of a novel  
single-phase red emitting phosphor  $\text{CaSr}_2(\text{PO}_4)_2: \text{Sm}^{3+}, \text{Li}^+$**

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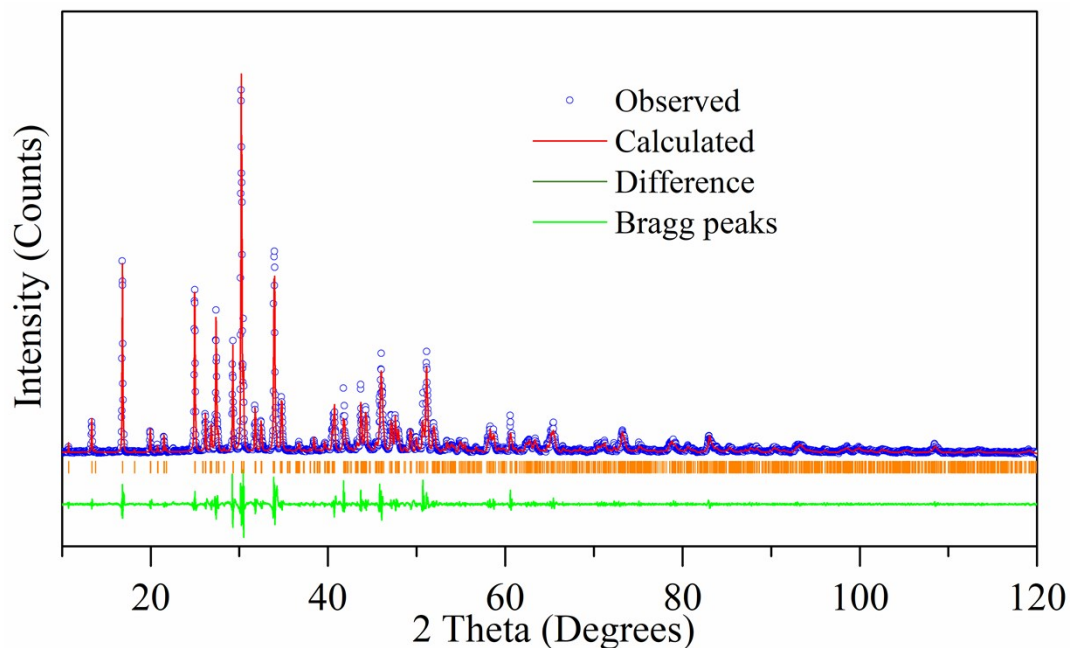


Fig. S1 The Rietveld refinement of  $\text{CaSr}_{1.82}\text{Sm}_{0.09}\text{Li}_{0.09}(\text{PO}_4)_2$  by TOPAS program. Solid red lines are calculated intensities, and blue circles are the observed intensities. Short orange vertical lines show the position of Bragg reflections of the calculated pattern. Green solid lines below the profiles stand for the difference between the observed and the calculated intensities.

Table S1. Crystallographic data for  $\text{CaSr}_{1.82}\text{Sm}_{0.09}\text{Li}_{0.09}(\text{PO}_4)_2$  based on Rietveld refinement.

Formula	$\text{CaSr}_{1.82}\text{Sm}_{0.09}\text{Li}_{0.09}(\text{PO}_4)_2$
Space group	<i>R3c</i> (161)
Symmetry	<i>Trigonal</i>
a/b(Å)	10.5918(11)
c(Å)	38.835(4)
$\alpha/\beta$	90°
$\gamma$	120°
$V(\text{Å}^3)$	3773.06(55)
$R_{wp}(\%)$	15.47
$R_p(\%)$	10.64
$\chi^2$	7.757

Table S2. The refined atomic positions and isotropic temperature factors for all atoms.

Atom	Wyckoff position	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}$
Ca1	18 <i>b</i>	0.7254(24)	0.8510(31)	0.1923(8)	0.040(9)
Sr1	18 <i>b</i>	0.7254(24)	0.8510(31)	0.1923(8)	0.040(9)
Sm1	18 <i>b</i>	0.7254(24)	0.8510(31)	0.1923(8)	0.040(9)
Li1	18 <i>b</i>	0.7254(24)	0.8510(31)	0.1923(8)	0.040(9)
Ca2	18 <i>b</i>	0.6320(25)	0.8104(31)	-0.0111(7)	0.015(7)
Sr2	18 <i>b</i>	0.6320(25)	0.8104(31)	-0.0111(7)	0.015(7)
Sm2	18 <i>b</i>	0.6320(25)	0.8104(31)	-0.0111(7)	0.015(7)
Li2	18 <i>b</i>	0.6320(25)	0.8104(31)	-0.0111(7)	0.015(7)
Ca3	18 <i>b</i>	0.7075(24)	0.8628(25)	0.0879(8)	0.016(5)
Sr3	18 <i>b</i>	0.7075(24)	0.8628(25)	0.0879(8)	0.016(5)
Sm3	18 <i>b</i>	0.7075(24)	0.8628(25)	0.0879(8)	0.016(5)
Li3	18 <i>b</i>	0.7075(24)	0.8628(25)	0.0879(8)	0.016(5)
Ca4	6 <i>a</i>	0	0	-0.07723	0.0126
Sr4	6 <i>a</i>	0	0	-0.07723	0.0126
Sm4	6 <i>a</i>	0	0	-0.07723	0.0126
Li4	6 <i>a</i>	0	0	-0.07723	0.0126
Ca5	6 <i>a</i>	0	0	0.75595	0.0504
P1	6 <i>a</i>	0	0	0	0.0589
P2	18 <i>b</i>	0.72429	0.84177	0.88810	0.0269
P3	18 <i>b</i>	0.65703	0.83698	0.79027	0.0474
O1	18 <i>b</i>	0.74948	-0.14214	-0.06854	-0.0301
O2	18 <i>b</i>	0.77933	0.75582	0.88544	0.0428
O3	18 <i>b</i>	0.65657	0.04995	0.87126	0.1265
O4	18 <i>b</i>	0.59511	0.87538	0.89581	0.0702
O5	18 <i>b</i>	0.61718	-0.11692	0.79938	0.1148
O6	18 <i>b</i>	0.60509	0.63715	0.81502	0.0256
O7	18 <i>b</i>	0.09528	0.91418	0.79922	-0.0512
O8	18 <i>b</i>	0.62949	0.81201	0.74855	0.0803
O9	18 <i>b</i>	-0.03498	0.85258	-0.01338	0.0158
O10	6 <i>a</i>	0	0	0.04823	0.0197