Supporting Information

Effect of Al/Si Substitution on the Structure and Luminescence Properties of $CaSrSiO_4:Ce^{3+}$ Phosphor: Analysis based on the Polyhedral Distortion†

Shihai Miao[1], Zhiguo Xia[2,*], Maxim S. Molokeev[3,4], Mingyue Chen, Jie Zhang[1], Quanlin Liu[2]

[1]*School of Materials Sciences and Technology, China University of Geosciences, Beijing 100083, China*

[2]*School of Materials Sciences and Engineering, University of Science and Technology Beijing, Beijing 100083, China*

[3]*Laboratory of Crystal Physics, Kirensky Institute of Physics, SB RAS, Krasnoyarsk 660036, Russia*

[4]*Department of Physics, Far Eastern State Transport University, Khabarovsk, 680021 Russia*

Table S1 Fractional atomic coordinates and isotropic displacement parameters (Å^2) of $(Ca_{0.95}Sr_{0.95}Ce_{0.05}Li_{0.05})(Si_{1-x}Al_x)O_4$.

	x	*y*	*z*	B_{iso}	Occ.
$(Ca_{0.95}Sr_{0.95}Ce_{0.05}Li_{0.05})(Si_{1-x}Al_x)O_4$, *x*=0					
Ca1	0.3376 (4)	0.25 (8)	0.5769 (3)	1.00 (12)	0.117 (5)
Sr1	0.3376 (4)	0.25 (8)	0.5769 (3)	1.00 (12)	0.358 (5)
Ce1	0.3376 (4)	0.25 (8)	0.5769 (3)	1.00 (12)	0.0125
Li1	0.3376 (4)	0.25 (8)	0.5769 (3)	1.00 (12)	0.0125
Ca2	0.9958 (5)	0.266 (4)	0.3026 (4)	1.0 (2)	0.358 (5)
Sr2	0.9958 (5)	0.266 (4)	0.3026 (4)	1.0 (2)	0.117 (5)
Ce2	0.9958 (5)	0.266 (4)	0.3026 (4)	1.0 (2)	0.0125
Li2	0.9958 (5)	0.266 (4)	0.3026 (4)	1.0 (2)	0.0125
Si	0.7796 (9)	0.25	0.5820 (11)	1.0 (2)	1
O1	1.013 (2)	0.315 (4)	0.5687 (16)	1.5 (3)	0.5
O2	0.744 (4)	0.024 (6)	0.688 (3)	1.5 (3)	0.5
O3	0.671 (2)	0.212 (5)	0.4363 (17)	1.5 (3)	0.5
O4	0.703 (4)	0.494 (6)	0.656 (3)	1.5 (3)	0.5
$(Ca_{0.95}Sr_{0.95}Ce_{0.05}Li_{0.05})(Si_{1-x}Al_x)O_4$, *x*=0.01					

Ca1	0.3367 (3)	0.239 (3)	0.5769 (3)	1.0 (1)	0.096 (4)
Sr1	0.3367 (3)	0.239 (3)	0.5769 (3)	1.0 (1)	0.379 (4)
Ce1	0.3367 (3)	0.239 (3)	0.5769 (3)	1.0 (1)	0.0125
Li1	0.3367 (3)	0.239 (3)	0.5769 (3)	1.0 (1)	0.0125
Ca2	0.9954 (5)	0.275 (2)	0.3003 (4)	1.0 (2)	0.379 (4)
Sr2	0.9954 (5)	0.275 (2)	0.3003 (4)	1.0 (2)	0.096 (4)
Ce2	0.9954 (5)	0.275 (2)	0.3003 (4)	1.0 (2)	0.0125
Li2	0.9954 (5)	0.275 (2)	0.3003 (4)	1.0 (2)	0.0125
Si	0.7738 (8)	0.25	0.581 (1)	1.25 (17)	0.99
Al	0.7738 (8)	0.25	0.581 (1)	1.25 (17)	0.01
O1	1.001 (2)	0.316 (3)	0.5702 (14)	1.5 (2)	0.5
O2	0.739 (4)	0.022 (5)	0.688 (3)	1.5 (2)	0.5
O3	0.660 (2)	0.208 (4)	0.4377 (14)	1.5 (2)	0.5
O4	0.706 (4)	0.503 (5)	0.656 (3)	1.5 (2)	0.5
$(Ca_{0.95}Sr_{0.95}Ce_{0.05}Li_{0.05})(Si_{1-x}Al_x)O_4$, x=0.1					
Ca1	0.3372 (3)	0.247 (12)	0.5781 (3)	1.0 (1)	0.114 (4)
Sr1	0.3372 (3)	0.247 (12)	0.5781 (3)	1.0 (1)	0.361 (4)
Ce1	0.3372 (3)	0.247 (12)	0.5781 (3)	1.0 (1)	0.0125
Li1	0.3372 (3)	0.247 (12)	0.5781 (3)	1.0 (1)	0.0125

Ca2	0.9934 (4)	0.270 (3)	0.2993 (3)	1.00 (18)	0.361 (4)
Sr2	0.9934 (4)	0.270 (3)	0.2993 (3)	1.00 (18)	0.114 (4)
Ce2	0.9934 (4)	0.270 (3)	0.2993 (3)	1.00 (18)	0.0125
Li2	0.9934 (4)	0.270 (3)	0.2993 (3)	1.00 (18)	0.0125
Si	0.7767 (8)	0.25	0.5848 (8)	1.16 (16)	0.9
Al	0.7767 (8)	0.25	0.5848 (8)	1.16 (16)	0.1
O1	1.0042 (18)	0.320 (3)	0.5564 (12)	1.5 (2)	0.5
O2	0.737 (4)	0.014 (5)	0.688 (3)	1.5 (2)	0.5
O3	0.6549 (18)	0.206 (4)	0.4327 (13)	1.5 (2)	0.5
O4	0.699 (4)	0.485 (5)	0.656 (3)	1.5 (2)	0.5