

## New $\text{Y}_2\text{LuCaAl}_2\text{SiO}_{12}:\text{Ln}$ ( $\text{Ln} = \text{Ce}^{3+}, \text{Eu}^{3+}$ , and $\text{Tb}^{3+}$ ) phosphors for white LEDs applications

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Table S1. Calculated positional parameter ( $x$ ,  $y$ ) of the screened compounds.

	Compositions	Annealing temperature (°C)	$x$	$y$	Phase <sup>a)</sup>	Selection
1	$\text{Y}_2\text{LuMgAl}_2\text{SiO}_{12}$	1400	0.0331	0.0522	$\text{Lu}_2\text{O}_3 + \text{Y}_2\text{O}_3 + \text{Al}_2\text{O}_3 + \text{unknown}$	X
2	$\text{Y}_2\text{LuCaAl}_3\text{SiO}_{12}$	1400	0.0348	0.0550	$\text{Lu}_2\text{O}_3 + \text{Y}_2\text{O}_3 + \text{Al}_2\text{O}_3 + \text{unknown}$	X
3	$\text{Y}_2\text{LuMgGaAl}_2\text{SiO}_{12}$	1400	0.0336	0.0530	$\text{Lu}_2\text{O}_3 + \text{Y}_4\text{Al}_3\text{O}_9 + \text{Lu}_4\text{Al}_2\text{O}_9 + \text{Y}_2\text{Si}_2\text{O}_7 + \text{unknown}$	X
4	<b><math>\text{Y}_2\text{LuCaGaAl}_2\text{SiO}_{12}</math></b>	<b>1600</b>	<b>0.0353</b>	<b>0.0558</b>	<b>YAG type garnet structure + <math>\text{YAlO}_3 + \text{CaAl}_2\text{Si}_2\text{O}_7 + \text{Ca}_2\text{Ga}_2\text{SiO}_7</math></b>	O
5	$\text{Y}_2\text{LuMgAl}_3\text{TiO}_{12}$	1400	0.0305	0.0539	$\text{Lu}_2\text{O}_3 + \text{Y}_2\text{O}_3 + \text{Lu}_4\text{Al}_2\text{O}_9 + \text{Al}_2\text{O}_3 + \text{unknown}$	X
6	$\text{Y}_2\text{LuMgGaAl}_2\text{TiO}_{12}$	1400	0.0310	0.0547	$\text{Lu}_2\text{O}_3 + \text{Y}_4\text{Al}_3\text{O}_9 + \text{Lu}_4\text{Al}_2\text{O}_9 + \text{MgY}_4\text{Si}_3\text{O}_{13} + \text{unknown}$	X
7	$\text{Y}_2\text{LuMgGa}_3\text{ZrO}_{12}$	1400	0.0274	0.0568	$\text{MgY}_4\text{Si}_3\text{O}_{13} + \text{Ca}_2\text{SiO}_4 + \text{Zr}_{0.82}\text{Y}_{0.18}\text{O}_{1.91} + \text{Y}_2\text{O}_3 + \text{MgO}_4 + \text{ZrO}_2 + \text{unknown}$	X
8	<b><math>\text{Y}_2\text{LaCaGa}_3\text{ZrO}_{12}</math></b>	<b>1400</b>	<b>0.0291</b>	<b>0.0596</b>	<b>Garnet structure + <math>\text{Y}_2\text{O}_3</math></b>	O
9	$\text{Y}_2\text{GdMgGaAl}_2\text{ZrO}_{12}$	1400	0.0290	0.0559	Melted	X
10	$\text{La}_2\text{LuCa}_2\text{Al}_2\text{VO}_{12}$	1100	0.0387	0.0584	$\text{LaAlO}_3 + \text{Lu}_2\text{O}_3 + \text{CaVO}_3 + \text{Ca}_8\text{La}_2\text{V}_6\text{O}_{26}$	X
11	$\text{Na}_2\text{LaMg}_2\text{P}_3\text{O}_{12}$	1100	0.0474	0.0444	$\text{LaPO}_4 + \text{CaLaAl}_3\text{O}_7 + \text{CaV}_2\text{O}_5$	X

12	$\text{Na}_2\text{LaCa}_2\text{PV}_2\text{O}_{12}$	1100	0.0449	0.0539	$\text{La}_2\text{O}_3 + \text{AlV}_3\text{O}_9 + \text{LaCa}_2\text{V}_3\text{O}_{9.74}$	X
13	$\text{NaCa}_2\text{Mg}_2\text{P}_3\text{O}_{12}$	1100	0.0465	0.0451	$\text{Ca}_9\text{MgNa}(\text{PO}_4)_7 + \text{La}_3\text{VO}_7$	X
14	$\text{Ca}_2\text{Mg}_2\text{GaSi}_2\text{PO}_{12}$	1100	0.0355	0.0525	$\text{Ca}_7\text{Mg}_2\text{P}_6\text{O}_{24} + \text{MgGa}_2\text{O}_4 + \text{CaGa}_2\text{O}_6$	X
15	$\text{Ca}_3\text{AlVP}_2\text{O}_{12}$	1100	0.0407	0.0439	$\text{Ca}_9\text{Al}(\text{PO}_4)_7 + \text{Ca}_3(\text{PO}_4)_2$	X
16	$\text{Ca}_3\text{GaVP}_2\text{O}_{12}$	1100	0.0417	0.0456	$\text{Ca}_9\text{Ga}(\text{PO}_4)_7 + \text{CaVO}_3 + \text{Ca}_3\text{Ga}_4\text{O}_9$	X
17	$\text{Ca}_2\text{LaMg}_2\text{AlP}_2\text{O}_{12}$	1100	0.0413	0.0489	$\text{CaLaAl}_3\text{O}_7 + \text{LaAlO}_3 + \text{CaAl}_2\text{O}_6 + \text{Ca}_4\text{V}_2\text{O}_9 + \text{CaMgP}_2\text{O}_7$	X
18	$\text{Ca}_2\text{LuCa}_2\text{GaVPO}_{12}$	1100	0.0402	0.0575	$\text{Lu}_8\text{V}_2\text{O}_{17} + \text{V}_2\text{GaO}_5 + \text{Lu}_2\text{O}_3 + \text{CaAl}_2\text{O}_3$	X
19	$\text{Ca}_2\text{LuZn}_2\text{Zr}_2\text{VO}_{12}$	1100	0.0246	0.0606	$\text{Ca}_2\text{Zr}_7\text{O}_{16} + \text{Lu}_2\text{O}_3 + \text{CaV}_3\text{O}_7 + \text{LaVO}_4$	X
20	$\text{La}_2\text{GdCaAl}_3\text{SiO}_{12}$	1400	0.0381	0.0521	$\text{LaAlO}_3 + \text{unknown}$	X
21	$\text{Gd}_3\text{MgAl}_3\text{TiO}_{12}$	1400	0.0318	0.0527	$\text{Gd}_2\text{Ti}_2\text{O}_7 + \text{Gd}_2\text{O}_3 + \text{unknown}$	X
22	$\text{Ca}_2\text{LaMg}_2\text{AlP}_2\text{O}_{12}$	1400	0.0427	0.0476	$\text{LaAlO}_3 + \text{LaPO}_4 + \text{AlPO}_4 + \text{Ca}_3(\text{PO}_4)_2$	X
23	$\text{Na}_7\text{Y}_3\text{Zr}_2\text{O}_{12}$	1200	0.0295	0.0613	$\text{Y}_2\text{O}_3 + \text{Na}_2\text{ZrO}_3 + \text{unknown}$	X
24	$\text{Na}_3\text{Ca}_2\text{Lu}_3\text{Zr}_2\text{O}_{12}$	1200	0.0284	0.0610	$\text{Lu}_2\text{O}_3 + \text{CaZrO}_3 + \text{unknown}$	X
25	$\text{Li}_3\text{Gd}_3\text{Ca}_2\text{Zr}_2\text{O}_{12}$	1200	0.0272	0.0663	$\text{CaMgP}_2\text{O}_7 + \text{LaAlO}_3 + \text{unknown}$	X
26	$\text{Li}_4\text{Na}_3\text{Lu}_3\text{Zr}_2\text{O}_{12}$	1200	0.0284	0.0605	$\text{Zr}_{0.82}\text{Y}_{0.18}\text{O}_{1.91} + \text{Lu}_2\text{O}_3 + \text{unknown}$	X
27	$\text{Ca}_2\text{NaY}_3\text{Zr}_2\text{O}_{12}$	1200	0.0284	0.0622	$\text{Y}_2\text{O}_3 + \text{Ca}_2\text{Zr}_7\text{O}_{16} + \text{unknown}$	X

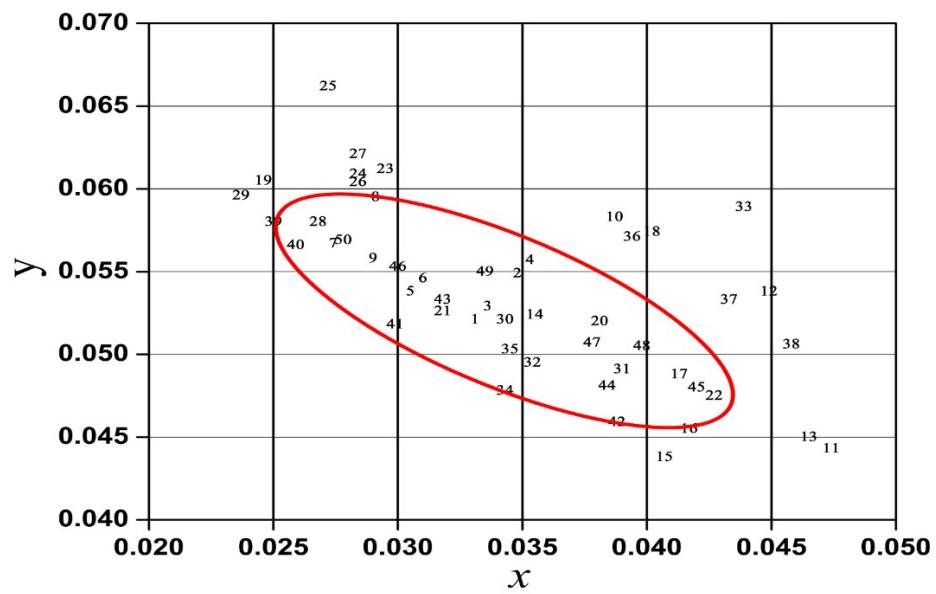
<b>28</b>	<b>Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub></b>	<b>980</b>	<b>0.0268</b>	<b>0.0581</b>	<b>Garnet structure</b>	O
29	Y <sub>2</sub> LaMg <sub>2</sub> GaZr <sub>2</sub> O <sub>12</sub>	1200	0.0237	0.0597	Y <sub>2</sub> O <sub>3</sub> + ZrO <sub>2</sub> + Y <sub>4</sub> Ga <sub>2</sub> O <sub>9</sub> + La <sub>2</sub> Zr <sub>2</sub> O <sub>2</sub> + unknown	X
30	La <sub>3</sub> Mg <sub>2</sub> GaZrSiO <sub>12</sub>	1400	0.0343	0.0522	La <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> + Li <sub>9.33</sub> Si <sub>6</sub> O <sub>26</sub> + Ga <sub>2</sub> O <sub>3</sub> + unknown	X
31	Gd <sub>3</sub> MgGaVPO <sub>12</sub>	1200	0.0390	0.0492	Mg <sub>2</sub> VO <sub>4</sub> + ZrO <sub>2</sub> + (VO) <sub>2</sub> P <sub>2</sub> O <sub>7</sub>	X
<b>32</b>	<b>LaNaCaGa<sub>3</sub>PZrO<sub>12</sub></b>	<b>1300</b>	<b>0.0354</b>	<b>0.0496</b>	<b>Garnet structure</b>	O
33	Ca <sub>3</sub> Lu <sub>2</sub> P <sub>2</sub> VO <sub>12</sub>	1100	0.0439	0.0590	Lu <sub>2</sub> O <sub>3</sub> + Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> + CaP <sub>2</sub> O <sub>6</sub>	X
34	Na <sub>2</sub> Ca <sub>2</sub> Al <sub>3</sub> PZrO <sub>12</sub>	1200	0.0343	0.0479	ZrO <sub>2</sub> + AlPO <sub>4</sub> + unknown	X
35	Ca <sub>3</sub> Ga <sub>3</sub> PZrO <sub>12</sub>	1200	0.0345	0.0504	CaZrO <sub>3</sub> + ZrO <sub>2</sub> + CaGa <sub>4</sub> O <sub>7</sub> + unknown	X
36	Ca <sub>3</sub> Lu <sub>2</sub> Si <sub>2</sub> ZrO <sub>12</sub>	1200	0.0394	0.0572	Lu <sub>2</sub> O <sub>3</sub> + ZrO <sub>2</sub> + CaZrO <sub>3</sub> + Ca <sub>2</sub> SiO <sub>4</sub> + unknown	X
37	NaCa <sub>2</sub> Gd <sub>2</sub> Si <sub>2</sub> VO <sub>12</sub>	1200	0.0433	0.0534	Ca <sub>2</sub> Gd <sub>8</sub> (SiO <sub>4</sub> ) <sub>6</sub> O <sub>2</sub> + Ca <sub>2</sub> SiO <sub>4</sub> + unknown	X
38	NaCa <sub>2</sub> Y <sub>2</sub> Si <sub>2</sub> PO <sub>12</sub>	1200	0.0458	0.0507	NaY <sub>9</sub> Si <sub>6</sub> O <sub>26</sub> + Na <sub>2</sub> CaPO <sub>4</sub> + unknown	X
39	Ca <sub>3</sub> Mg <sub>2</sub> Ga <sub>2</sub> Zr <sub>2</sub> O <sub>12</sub>	1200	0.0250	0.0581	CaZrO <sub>3</sub> + Ca <sub>3</sub> Ga <sub>4</sub> O <sub>9</sub> + MgGa <sub>2</sub> O <sub>4</sub> + Ga <sub>2</sub> O <sub>3</sub>	X
40	Y <sub>2</sub> CaMgAl <sub>2</sub> Zr <sub>2</sub> O <sub>12</sub>	1200	0.0259	0.0567	ZrO <sub>2</sub> + Y <sub>2</sub> O <sub>3</sub> + CaZrO <sub>3</sub> + Al <sub>2</sub> O <sub>3</sub> + unknown	X
41	Lu <sub>2</sub> MgAl <sub>2</sub> V <sub>2</sub> O <sub>12</sub>	1200	0.0299	0.0519	LuVO <sub>4</sub> + unknown	X

42	$\text{Lu}_2\text{MgAl}_2\text{P}_2\text{O}_{12}$	1200	0.0388	0.0460	Melted	X
43	$\text{Gd}_2\text{CaMgGa}_2\text{Ti}_2\text{O}_{12}$	1200	0.0318	0.0534	$\text{CaTiO}_3 + \text{Gd}_3\text{Ga}_5\text{O}_{12} + \text{GdTiO}_3 + \text{GdTiO}_3 + \text{unknown}$	X
44	$\text{Y}_2\text{CaGa}_2\text{PVO}_{12}$	1200	0.0384	0.0482	$\text{Y}_3\text{Ga}_5\text{O}_{12} + \text{Ga}_2\text{O}_3 + \text{YVO}_4 + \text{Ca}_3\text{Y}_2\text{O}_6 + \text{CaV}_2\text{O}_6 + \text{unknown}$	X
45	$\text{NaCa}_2\text{Mg}_2(\text{V, P})_3\text{O}_{12}$	1200	0.0420	0.0481	$\text{NaCa}_2\text{Mg}_2(\text{VO}_4)_3 + \text{Ca}_7\text{Mg}_2\text{P}_6\text{O}_{24} + \text{unknown}$	X
46	$\text{K}_2\text{Ca}_3\text{Mg}_2\text{Zr}_3\text{O}_{12}$	1200	0.0300	0.0554	$\text{CaZrO}_3 + \text{CaMgP}_2\text{O}_7 + \text{unknown}$	X
47	$\text{NaCaNb}_2\text{V}_3\text{O}_{12}$	1200	0.0378	0.0508	Melted	X
48	$\text{LiCa}_2\text{Zn}_2(\text{P, V})_3\text{O}_{12}$	1200	0.0398	0.0506	$\text{Ca}_2\text{P}_2\text{O}_7 + \text{Ca}_{10}\text{Li}(\text{PO}_4)_7 + \text{LiCaP}_3\text{O}_9 + \text{unknown}$	X
49	$\text{NaMg}_2\text{Zn}_2\text{V}_3\text{O}_{12}$	1200	0.0335	0.0551	Melted	X
50	$\text{Y}_2\text{LaMg}_2\text{GaZrTiO}_{12}$	1200	0.0278	0.0570	$\text{Zr}_{0.82}\text{Y}_{0.18}\text{O}_{1.91} + \text{La}_2\text{MgTiO}_6 + \text{MgTiO}_3 + \text{unknown}$	X

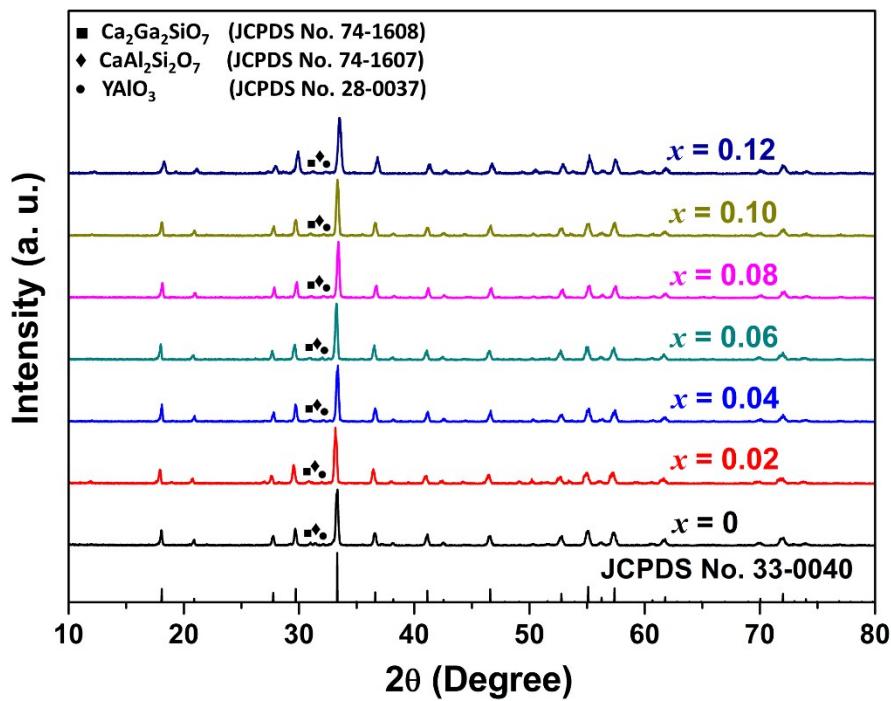
a)The phase was obtained from XRD results.

Table S2. Calculated amount of the impurities present in the  $\text{Y}_{2-x}\text{LuCaGaAl}_2\text{SiO}_{12}:\text{xEu}^{3+}$  phosphors

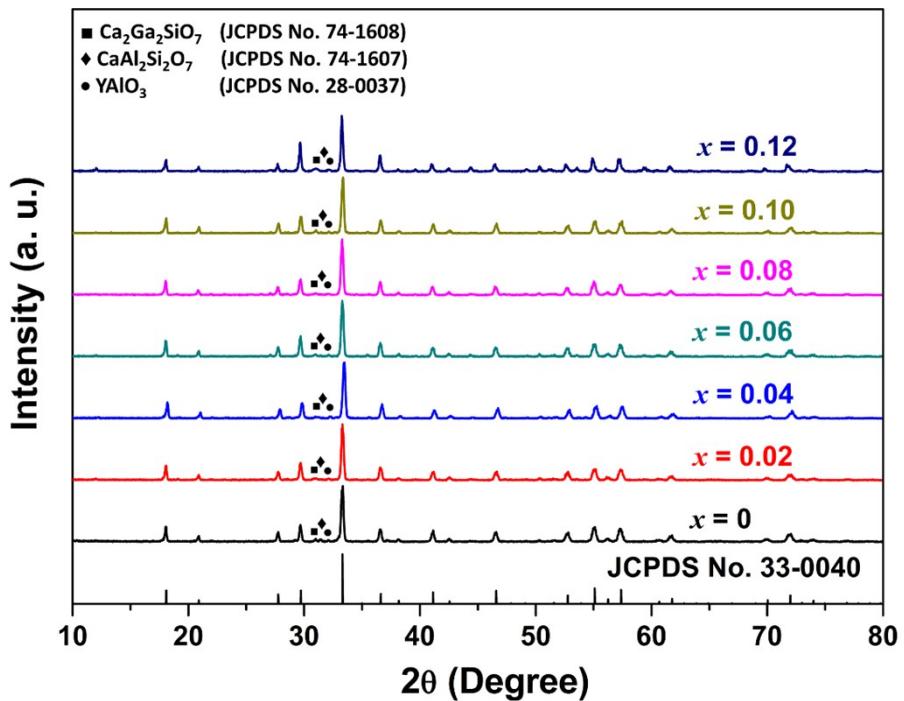
Content (x)	Integrated intensity			Integrated intensity of Main peak ( $\Sigma D$ )	Total impurity (X= A+B+C)	$\frac{X}{\Sigma D} \times 100(\%)$
	$\text{Ca}_2\text{Ga}_2\text{SiO}_7$ (A)	$\text{CaAl}_2\text{Si}_2\text{O}_7$ (B)	$\text{YAlO}_3$ (C)			
$x = 0$	0.017	0.013	0.007	1.219	0.037	3.03
$x = 0.02$	0.025	0.009	0.006	1.09	0.04	3.67
$x = 0.04$	0.019	0.010	0.008	1.057	0.037	3.50
$x = 0.06$	0.020	0.010	0.007	1.062	0.037	3.48
$x = 0.08$	0.017	0.012	0.009	1.088	0.038	3.49
$x = 0.10$	0.025	0.015	0.006	1.567	0.046	2.94
$x = 0.12$	0.037	0.021	0.004	1.649	0.062	3.76



**Fig. S1.** Plot of the positional coordinate ( $x, y$ ) calculated from the designed garnet compounds.



**Fig. S2.** XRD patterns of the  $\text{Y}_{2-x}\text{LuCaGaAl}_2\text{SiO}_{12}:x\text{Eu}^{3+}$  ( $0 \leq x \leq 0.12$ ) phosphors.



**Fig. S3.** XRD patterns of the  $\text{Y}_{2-x}\text{LuCaGaAl}_2\text{SiO}_{12}:x\text{Tb}^{3+}$  ( $0 \leq x \leq 0.12$ ) phosphors.