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Thermal-stability Synergy Improvement of Sm^{3+} and Eu^{3+} in $Ca_{3.6}In_{3.6}(PO_4)_6$: the Effect of Local Symmetry

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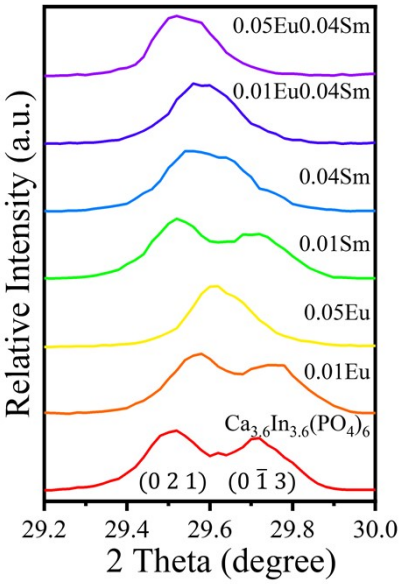

Figure S1 The XRD magnification in 2-Theta range between 29.2° and 30° in **Figure 1(a).**

Table S1 Rietveld refinement for the $CI_{1-x}P$: $0.05Eu^{3+}$, $CI_{1-y}P$: $0.04Sm^{3+}$, and $CI_{1-x-y}P$: $0.05Eu^{3+}$, $0.04Sm^{3+}$.

Formula	$Ca_{3.420}Eu_{0.180}In_{3.6}(PO_4)_6$	$Ca_{3.456}Sm_{0.144}In_{3.6}(PO_4)_6$	$Ca_{3.276}Sm_{0.144}Eu_{0.180}In_{3.6}(PO_4)_6$
Sample	Multi-crystal powder	Multi-crystal powder	Multi-crystal powder
R_B (%)	6.31	6.49	5.70
Rp (%)	7.37	7.32	7.10
R_{WP} (%)	9.76	9.74	9.36
S	2.20	2.28	2.36
Symmetry	Triclinic	Triclinic	Triclinic
Space group	P $\bar{1}$ (No.2)	P $\bar{1}$ (No.2)	P $\bar{1}$ (No.2)
a (Å)	6.5001(1)	6.4977(1)	6.5047(1)
b (Å)	9.1903(1)	9.1973(1)	9.1753(1)

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c (Å)	9.2899(1)	9.2798(1)	9.3149(1)
α (°)	110.9844(6)	110.9799(7)	111.0247(6)
β (°)	101.3658(7)	101.3440(8)	101.3663(7)
γ (°)	108.2570(7)	108.2461(8)	108.2853(7)
V (Å^3)	461.17(1)	460.99(1)	461.67(1)
Z	2	2	2
Calculated density (g/cm^3)	4.08	4.08	4.10

Table S2 Atomic parameters for $CI_{1-x}P$: $0.05Eu^{3+}$.

Atom	x	y	z	Wyck.	OCC.	U (Å^2)
O1	0.1752(19)	0.7248(16)	0.0380(14)	2i	1	0.0007
O2	0.4064(20)	0.1730(15)	0.390(1)	2i	1	0.0007
O3	1.1097(17)	0.7683(13)	-0.4379(11)	2i	1	0.0023
O4	0.0233(16)	0.0092(6)	0.2042(14)	2i	1	0.0103
O5	0.968(2)	0.4963(15)	-0.6788(15)	2i	1	0.0075
O6	0.874(3)	0.7464(15)	-0.6694(15)	2i	1	0.0183
O7	0.409(3)	0.8389(17)	0.3151(11)	2i	1	0.0584
O8	0.400(2)	0.0747(17)	0.1173(15)	2i	1	0.0103
O9	0.232(2)	0.2886(7)	0.1871(5)	2i	1	0.0425
O10	0.520(2)	0.7880(17)	0.0663(16)	2i	1	0.0325
O11	0.6840(12)	0.5330(15)	-0.5720(12)	2i	1	0.0243
O12	0.655(2)	0.4576(6)	-0.1365(6)	2i	1	0.0435
P1	0.2611(9)	0.1284(7)	0.2199(6)	2i	1	0.0007
P2	0.9076(9)	0.6348(6)	-0.5954(6)	2i	1	0.0047
P3	0.3519(9)	0.7083(7)	0.1387(6)	2i	1	0.0012
Ca1	0.2186(8)	0.8298(6)	0.8401(5)	2i	1	0.001
Ca2	0.2624(14)	0.9953(12)	0.4977(10)	2i	0.80000	0.068
In1	0.8271(3)	0.7242(2)	0.0669(2)	2i	0.95498	0.017
Eu1	0.8271(3)	0.7242(2)	0.0669(2)	2i	0.04502	0.017
In2	0.6469(4)	0.4382(3)	-0.3853(2)	2i	0.75496	0.0082
Eu2	0.6469(4)	0.4382(3)	-0.3853(2)	2i	0.04488	0.0082

Table S3 Atomic parameters for $CI_{1-y}P$: $0.04Sm^{3+}$.

Atom	x	y	z	Wyck.	OCC.	U (Å^2)
O1	0.1762(18)	0.7206(16)	0.0410(14)	2i	1	0.0024
O2	0.3994(19)	0.1781(15)	0.3928(10)	2i	1	0.0024
O3	1.1076(17)	0.7705(13)	-0.4301(11)	2i	1	0.0024
O4	0.0332(17)	0.0096(6)	0.2060(14)	2i	1	0.0154
O5	0.967(2)	0.5018(14)	-0.6860(14)	2i	1	0.0083
O6	0.874(3)	0.7444(16)	-0.6730(17)	2i	1	0.0507
O7	0.425(3)	0.8484(17)	0.3215(11)	2i	1	0.0713
O8	0.396(2)	0.0685(16)	0.1076(14)	2i	1	0.0024
O9	0.234(2)	0.2883(7)	0.1867(5)	2i	1	0.0695
O10	0.514(2)	0.7988(18)	0.0676(17)	2i	1	0.0648
O11	0.6886(12)	0.5388(17)	-0.5675(14)	2i	1	0.0638
O12	0.346(2)	0.5428(6)	0.1341(5)	2i	1	0.0138
P1	0.2646(9)	0.1305(7)	0.2195(6)	2i	1	0.0077
P2	0.9146(9)	0.6379(6)	-0.5916(7)	2i	1	0.0135
P3	0.3628(10)	0.7153(7)	0.1444(6)	2i	1	0.015
Ca1	0.2252(8)	0.8258(6)	0.8409(5)	2i	1	0.0099
Ca2	0.2557(14)	0.9899(11)	0.4943(10)	2i	0.80000	0.0661
In1	0.8271(3)	0.7256(2)	0.0674(2)	2i	0.98450	0.0194
Sm1	0.8271(3)	0.7256(2)	0.0674(2)	2i	0.01550	0.0194
In2	0.6461(4)	0.4375(3)	-0.3836(2)	2i	0.74350	0.016
Sm2	0.6461(4)	0.4375(3)	-0.3836(2)	2i	0.05643	0.016

Table S4 Atomic parameters for $CI_{1-x-y}P$: $0.05Eu^{3+}$, $0.04Sm^{3+}$.

Atom	x	y	z	Wyck.	OCC	U [Å^2]
O1	0.1511(17)	0.7185(15)	0.0485(14)	2i	1	0.0156
O2	0.4087(20)	0.1793(16)	0.3903(10)	2i	1	0.0178
O3	1.1005(16)	0.7564(12)	-0.4408(10)	2i	1	0.0003
O4	0.0296(16)	0.0085(6)	0.1854(13)	2i	1	0.0228
O5	0.964(2)	0.4907(13)	-0.6874(13)	2i	1	0.0032
O6	0.864(2)	0.7316(14)	-0.6894(13)	2i	1	0.0069
O7	0.409(3)	0.8264(18)	0.3146(11)	2i	1	0.0987
O8	0.3888(19)	0.0702(15)	0.1055(12)	2i	1	0.0047
O9	0.222(2)	0.2945(7)	0.1840(5)	2i	1	0.0943
O10	0.529(2)	0.7941(18)	0.0837(17)	2i	1	0.0733
O11	0.6843(11)	0.5442(14)	-0.5641(11)	2i	1	0.0063
O12	0.356(2)	0.5417(6)	0.1395(6)	2i	1	0.0558
P1	0.2669(9)	0.1434(7)	0.2229(6)	2i	1	0.0198
P2	0.9057(9)	0.6304(6)	-0.5965(6)	2i	1	0.0124
P3	0.3539(10)	0.7130(7)	0.1418(7)	2i	1	0.0353
Ca1	0.2232(7)	0.8332(6)	0.8430(5)	2i	1	0.0034
Ca2	0.2554(15)	0.9923(12)	0.4893(11)	2i	0.80000	0.1106
In1	0.8259(3)	0.7255(2)	0.06998(20)	2i	0.91872	0.0349
Eu1	0.8259(3)	0.7255(2)	0.06998(20)	2i	0.03427	0.0349
Sm1	0.8259(3)	0.7255(2)	0.06998(20)	2i	0.04701	0.0349
In2	0.6513(4)	0.4366(3)	-0.3864(2)	2i	0.71925	0.0163
Eu2	0.6513(4)	0.4366(3)	-0.3864(2)	2i	0.05582	0.0163
Sm2	0.6513(4)	0.4366(3)	-0.3864(2)	2i	0.02494	0.0163

Table S5 The partial bond lengths (Å) of $CI_{1-x}P$: $0.05Eu^{3+}$, $CI_{1-y}P$: $0.04Sm^{3+}$, and $CI_{1-x-y}P$: $0.05Eu^{3+}$, $0.04Sm^{3+}$.

In1|Eu1	O12	x, y, z	2.2268	In2|Eu2	O11	x, y, z	2.2228
	O4	1+x, 1+y, z	2.2331		O11	1-x, 1-y, -1-z	2.2247
	O10	x, y, z	2.2494		O12	x, y, z	2.2423
	O9	1-x, 1-y, -z	2.2682		O9	1-x, 1-y, -z	2.2789
	O1	1+x, y, z	2.3291		O5	2-x, 1-y, -1-z	2.2792
	O6	x, y, 1+z	2.3333		O2	x, y, -1+z	2.3290
Average			2.2733	Average			2.2628
In1|Sm1	O12	1-x, 1-y, -z	2.2325	In2|Sm2	O11	1-x, 1-y, -1-z	2.2277
	O4	1+x, 1+y, z	2.2353		O11	x, y, z	2.2404
	O9	1-x, 1-y, -z	2.2623		O12	1-x, 1-y, -z	2.2457
	O6	x, y, 1+z	2.3035		O9	1-x, 1-y, -z	2.2837
	O10	x, y, z	2.3346		O5	2-x, 1-y, -1-z	2.2963
	O1	1+x, y, z	2.3417		O2	x, y, -1+z	2.3062
Average			2.2850	Average			2.2667
In1|Sm1|Eu1	O1	1+x, y, z	2.1739	In2|Eu2|Sm2	O11	1-x, 1-y, -1-z	2.2173
	O6	x, y, 1+z	2.1756		O11	x, y, z	2.2215
	O4	1+x, 1+y, z	2.2170		O12	1-x, 1-y, -z	2.2513
	O10	x, y, z	2.2190		O9	1-x, 1-y, -z	2.2591
	O12	1-x, 1-y, -z	2.2512		O5	2-x, 1-y, -1-z	2.2682
	O9	1-x, 1-y, -z	2.2570		O2	x, y, -1+z	2.2921
Average			2.2156	Average			2.2516

Table S6 The D values for $CI_{1-x}P$: $0.05Eu^{3+}$, $CI_{1-y}P$: $0.04Sm^{3+}$, and $CI_{1-x-y}P$: $0.05Eu^{3+}$, $0.04Sm^{3+}$ phosphors.

D	$CI_{1-x}P$: $0.05Eu^{3+}$	$CI_{1-y}P$: $0.04Sm^{3+}$	$CI_{1-x-y}P$: $0.05Eu^{3+}$, $0.04Sm^{3+}$
In1	0.0170	0.0182	0.0123
In2	0.0145	0.0127	0.0096
Average	0.01575	0.01545	0.01095

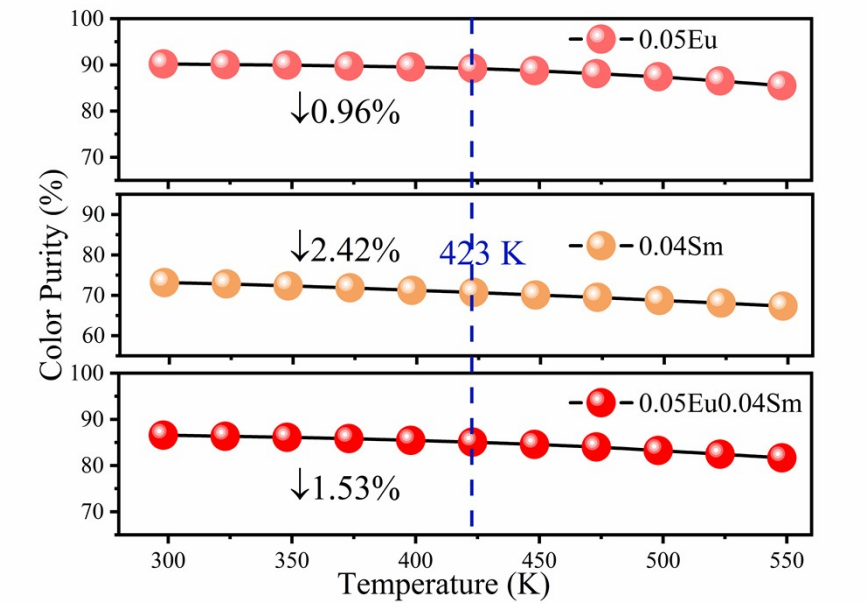

Figure S2 The color purity variation curve for $CI_{1-x}P$: $0.05Eu^{3+}$, $CI_{1-y}P$: $0.04Sm^{3+}$, and $CI_{1-x-y}P$: $0.05Eu^{3+}$, $0.04Sm^{3+}$ phosphors.

Table S7 The CIE and color purity of $CI_{1-x}P$: $0.05Eu^{3+}$ in different temperature.

Temperature (K)	(x, y)	CTT (K)	color purity (%)
298	(0.6419,0.3544)	7298	90.21
323	(0.6414,0.3547)	7205	90.05
348	(0.6411,0.3549)	7146	89.96
373	(0.6404,0.3554)	7007	89.75
398	(0.6398,0.3559)	6879	89.56
423	(0.6388,0.3567)	6676	89.25
448	(0.6372,0.3580)	6364	88.75
473	(0.6351,0.3595)	6008	88.09
498	(0.6330,0.3609)	5687	87.44
523	(0.6301,0.3626)	5303	86.54
548	(0.6267,0.3645)	4903	85.48
573	(0.6249,0.3661)	4652	84.90

Table S8 The CIE and color purity of $CI_{1-y}P$: $0.04Sm^{3+}$ in different temperature.

Temperature (K)	(x, y)	CTT (K)	color purity (%)
298	(0.5906,0.3956)	2217	73.15
323	(0.5897,0.3963)	2197	72.82
348	(0.5883,0.3972)	2159	72.33
373	(0.5870,0.3981)	2129	71.87
398	(0.5852,0.3993)	2091	71.23
423	(0.5838,0.4003)	2063	70.72
448	(0.5820,0.4015)	2031	70.08
473	(0.5804,0.4025)	2006	69.51
498	(0.5782,0.4036)	1978	68.74
523	(0.5765,0.4048)	1955	68.11
548	(0.5743,0.4060)	1933	67.33
573	(0.5725,0.4070)	1916	66.68

Table S9 The CIE and color purity of $CI_{1-x-y}P$: $0.05Eu^{3+}$, $0.04Sm^{3+}$ in different temperature.

Temperature (K)	(x,y)	CTT (K)	Color purity (%)
298	(0.6305,0.3646)	5117	86.60
323	(0.6297,0.3653)	4999	86.34
348	(0.6290,0.3660)	4890	86.11
373	(0.6282,0.3668)	4770	85.85
398	(0.6270,0.3679)	4605	85.45
423	(0.6258,0.3689)	4457	85.07
448	(0.6243,0.3701)	4285	84.58
473	(0.6226,0.3714)	4105	84.03
498	(0.6202,0.3729)	3892	83.26
523	(0.6178,0.3749)	3663	82.46
548	(0.6154,0.3764)	3482	81.69
573	(0.6134,0.3781)	3320	81.01