Anti-thermal Quenching Phosphors Based on the New Phosphate Host $Ca_{3.6}In_{3.6}(PO_4)_6$

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Table S1. Details of the Rietveld refinement results of CIP.

Parameter	Value
Sample	Multi-crystal powder
Formula	$Ca_{3.6}In_{3.6}(PO_4)_6$
R_B (%)	4.31
R_p (%)	2.61
R_{WP} (%)	3.59
S	2.24
Symmetry	Triclinic
Space group	$P\bar{1}$ (No.2)
a (Å)	6.4953(1)
b (Å)	9.2128(1)
c (Å)	9.2608(1)
α (°)	110.9441(7)
β (°)	101.3650(8)
γ (°)	108.2350(8)
V (Å3)	460.79(1)
Z	1
Calculated density (g/cm^3)	4.06

Table S2. Atomic parameters for CIP.

Atom	*x*	*y*	*z*	Wyck.	OCC.	U (Å^2)	CN
O1	0.1393(16)	0.7098(15)	0.0460(14)	2i	1	0.0000	3
O2	0.4029(20)	0.1862(15)	0.3989(10)	2i	1	0.0135	3
O3	1.1045(16)	0.7680(12)	-0.4455(11)	2i	1	0.0077	3
O4	0.0429(17)	0.0105(14)	0.2108(15)	2i	1	0.0210	4
O5	0.991(2)	0.5041(14)	-0.6824(14)	2i	1	0.0037	3
O6	0.877(3)	0.7341(16)	-0.6817(16)	2i	1	0.0278	4
O7	0.426(3)	0.8298(16)	0.3106(11)	2i	1	0.0888	3
O8	0.376(2)	0.0555(15)	0.0961(13)	2i	1	0.0041	3

O9	0.221(2)	0.2876(7)	0.1867(5)	2i	1	0.0284	4
O10	0.5371(17)	0.7674(16)	0.0708(14)	2i	1	0.0091	3
O11	0.6857(12)	0.5366(17)	-0.5682(13)	2i	1	0.0460	3
O12	0.636(2)	0.4480(12)	-0.1407(9)	2i	1	0.0162	3
P1	0.2633(9)	0.1331(7)	0.2193(6)	2i	1	0.0037	4
P2	0.9057(9)	0.6276(6)	-0.5953(6)	2i	1	0.0076	4
P3	0.3523(9)	0.7072(7)	0.1344(6)	2i	1	0.0096	4
Ca1	0.2284(8)	0.8262(6)	0.8447(6)	2i	1	0.0210	8
Ca2	0.2583(20)	0.9916(19)	0.4851(18)	2i	0.8	0.2071	7
In1	0.8285(3)	0.7258(2)	0.0659(2)	2i	1	0.0237	6
In2	0.6469(3)	0.4406(3)	-0.3819(2)	2i	0.8	0.0084	6

Table S3. The partial bond lengths (Å) and bond angles (Deg.) for the CIP.

P1	O4	1.4871	x, y, z
	O2	1.5408	x, y, z
	O8	1.5564	x, y, z
	O9	1.6468	x, y, z
Average		1.5578	
P2	O5	1.4720	x, y, z
	O3	1.4936	x, y, z
	O6	1.5015	x, y, z
	O11	1.5329	x, y, z
Average		1.5000	
P3	O1	x, y, z	1.4742
	O12	1-x, 1-y, -z	1.4763
	O10	x, y, z	1.4802
	O7	x, y, z	1.4845
Average		1.4788	
In1	O10	2.0511	x, y, z
	O1	2.1082	1+x, y, z
	O9	2.2501	1-x, 1-y, -z
	O4	2.2541	1+x, 1+y, z
	O6	2.2662	x, y, 1+z
	O12	2.3082	x, y, z
Average		2.2063	

Ca1	O8	2.2669	x, 1+y, 1+z
	O8	2.3143	1-x, 1-y, 1-z
	O3	2.4505	-1+x, y, 1+z
	O1	2.5350	x, y, 1+z
	O9	2.4899	-x, 1-y, 1-z
	O5	2.5684	1-x, 1-y, -z
	O4	2.6831	-x, 1-y, 1-z
	O10	2.9213	x, y, 1+z
Average		2.5634	
Ca2	O7	2.1507	1-x, 2-y, 1-z
	O2	2.2357	x, 1+y, z
	O2	2.304	x, 1+y, z
	O6	2.4509	-1+x, y, 1+z
	O7	2.4911	x, y, z
	O4	2.7402	x, 1+y, z
	O6	3.0339	1-x, 2-y, -z
Average		2.4985	
O4-P1-O2		96.852	
O4-P1-O8		117.812	
O4-P1-O9		101.504	
O2-P1-O8		112.154	
O2-P1-O9		114.847	
O8-P1-O9		107.639	
Average		109.464	
O5-P2-O3		107.165	
O5-P2-O6		111.096	
O5-P2-O11		107.560	

				O6-P2-O6	110.390
In2	O5	2.1511	2-x, 1-y, -1-z	O6-P2-O11	116.955
	O11	2.2101	1-x, 1-y, -1-z	O11-P2-O11	113.317
	O11	2.2238	x, y, z	Average	109.336
	O12	2.2261	x, y, z	O1-P3-O12	123.382
	O9	2.2544	1-x, 1-y, -z	O1-P3-O10	109.648
	O2	2.2653	x, y, -1+z	O1-P3-O7	107.198
				O12-P3-O10	104.033
Average		2.2218		O12-P3-O7	103.607
				O10-P3-O7	108.123
				Average	109.332

Table S4. The calculated valence states of each atoms in the CIP.

Atom	CN	Average distance	$V_{theo.}$	$V_{calc.}$	Error (%)
O1	3	2.0391	-2	2.259	12.95
O2	3	2.0142	-2	1.914	-4.30
O3	3	2.1010	-2	1.944	-2.80
O4	4	2.3043	-2	2.031	1.55
O5	3	2.0719	-2	2.072	3.60
O6	4	2.3294	-2	1.966	-1.70
O7	4	2.2035	-2	2.218	10.90
O8	3	2.0459	-2	2.014	0.70
O9	4	2.2104	-2	1.763	-11.85
O10	3	2.1509	-2	2.192	9.60
O11	3	1.9889	-2	1.938	-3.10
O12	3	2.0036	-2	2.129	6.45
P1	4	1.5578	5	4.749	-5.02
P2	4	1.5000	5	5.497	9.94
P3	4	1.4788	5	5.812	16.24
Ca1	8	2.5634	2	1.849	-7.55
Ca2	7	2.4985	2	2.112	5.60
In1	6	2.2063	3	2.725	-9.17
In2	6	2.2218	3	2.541	-15.30

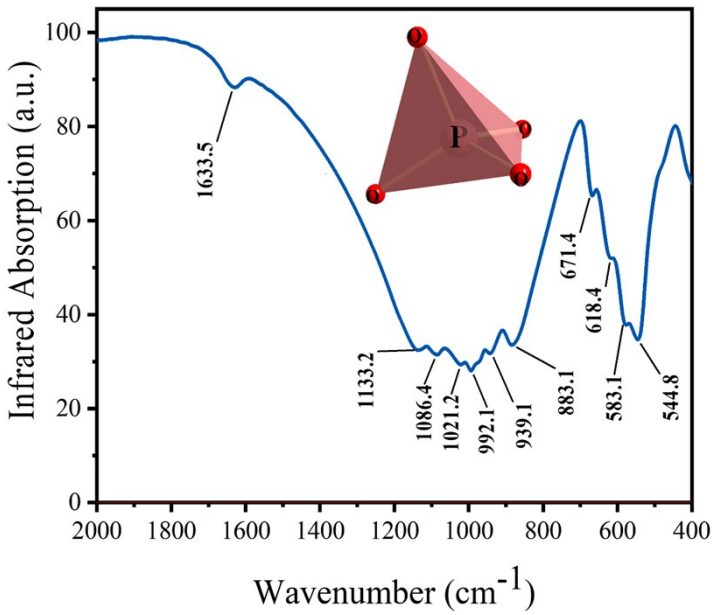

Figure S1. The Infrared spectroscopy of CIP from 400 to 2000 cm^{-1}.

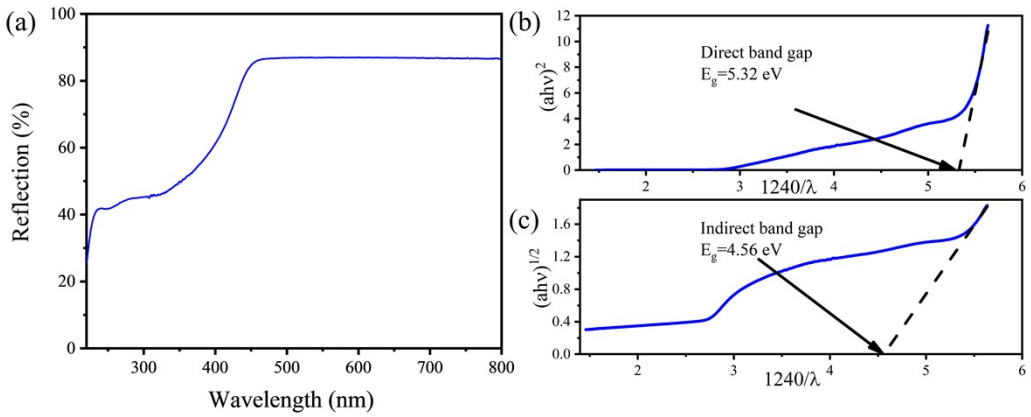

Figure S2. The diffuse reflectance spectra (a), extrapolation of the direct band gap (b) and indirect band gap (c) of CIP.

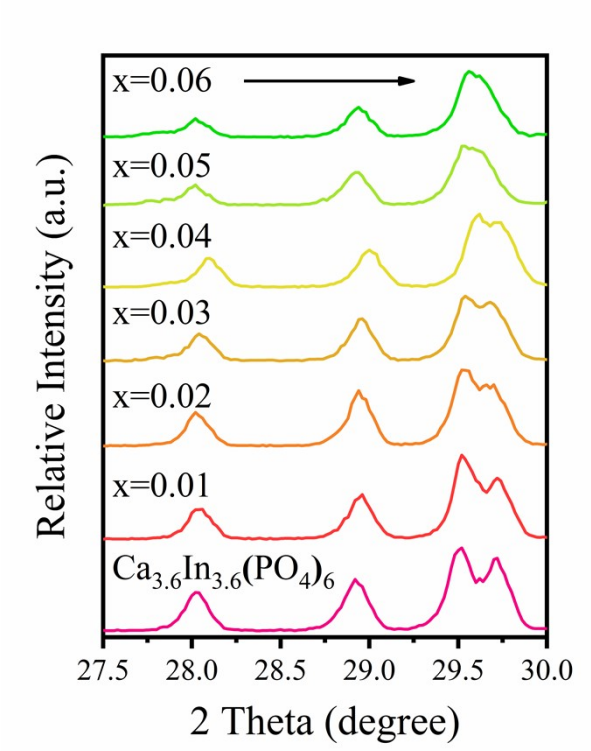

Figure S3. The XRD magnification between 27.5° and 30° for $C_{1-x}IP$: xDy^{3+}.

Table S5. Details of the Rietveld refinement results of $C_{1-x}IP$: $0.03Dy^{3+}$.

Parameter	Value
Formula	$Ca_{3.492}Dy_{0.108}In_{3.6}(PO_4)_6$
Sample	Multi-crystal powder
R_B(%)	8.13
R_p(%)	4.05
R_{WP}(%)	5.94
S	3.16
Symmetry	Triclinic
Space group	$P\bar{1}$ (No.2)
a (Å)	6.4938(1)
b (Å)	9.2015(2)
c (Å)	9.2683(1)
α (°)	110.9756(8)
β (°)	101.3388(9)
γ (°)	108.2376(9)
V (Å3)	460.43(1)
Z	1
Calculated density (g/cm^3)	4.11

Table S6. Atomic parameters for $C_{1-x}IP$: $0.03Dy^{3+}$.

Atom	*x*	*y*	*z*	Wyck.	OCC.	U (Å^2)
O1	0.1742(17)	0.7207(16)	0.0504(14)	2i	1	0.0000
O2	0.4098(19)	0.1886(15)	0.3992(10)	2i	1	0.0000
O3	1.1082(16)	0.7648(13)	-0.4390(11)	2i	1	0.0000
O4	0.0210(15)	0.0108(6)	0.1947(13)	2i	1	0.0059
O5	0.9818(9)	0.5060(12)	-0.6825(12)	2i	1	0.0000
O6	0.864(2)	0.7405(14)	-0.6854(8)	2i	1	0.0139
O7	0.425(3)	0.8597(17)	0.3172(12)	2i	1	0.0749
O8	0.398(2)	0.0796(19)	0.1134(16)	2i	1	0.0340
O9	0.234(3)	0.2908(8)	0.1914(6)	2i	1	0.1479
O10	0.5152(18)	0.7883(15)	0.0581(13)	2i	1	0.0000
O11	0.6944(14)	0.547(2)	-0.5619(18)	2i	1	0.1364
O12	0.656(2)	0.4587(6)	-0.1365(5)	2i	1	0.0206
P1	0.2655(9)	0.1362(7)	0.2278(6)	2i	1	0.0009
P2	0.9060(9)	0.6338(6)	-0.5972(6)	2i	1	0.0087
P3	0.3665(10)	0.7171(7)	0.1463(6)	2i	1	0.0185
Ca1	0.2248(8)	0.8224(6)	0.8398(6)	2i	0.95209	0.0299
Dy1	0.2248(8)	0.8224(6)	0.8398(6)	2i	0.04791	0.0299
Ca2	0.2585(14)	0.9913(12)	0.4943(10)	2i	0.79391	0.0679
Dy2	0.2585(14)	0.9913(12)	0.4943(10)	2i	0.00649	0.0679
In1	0.8261(3)	0.7260(2)	0.0645(2)	2i	1	0.0195
In2	0.6450(3)	0.4379(3)	-0.3865(2)	2i	0.8	0.0115

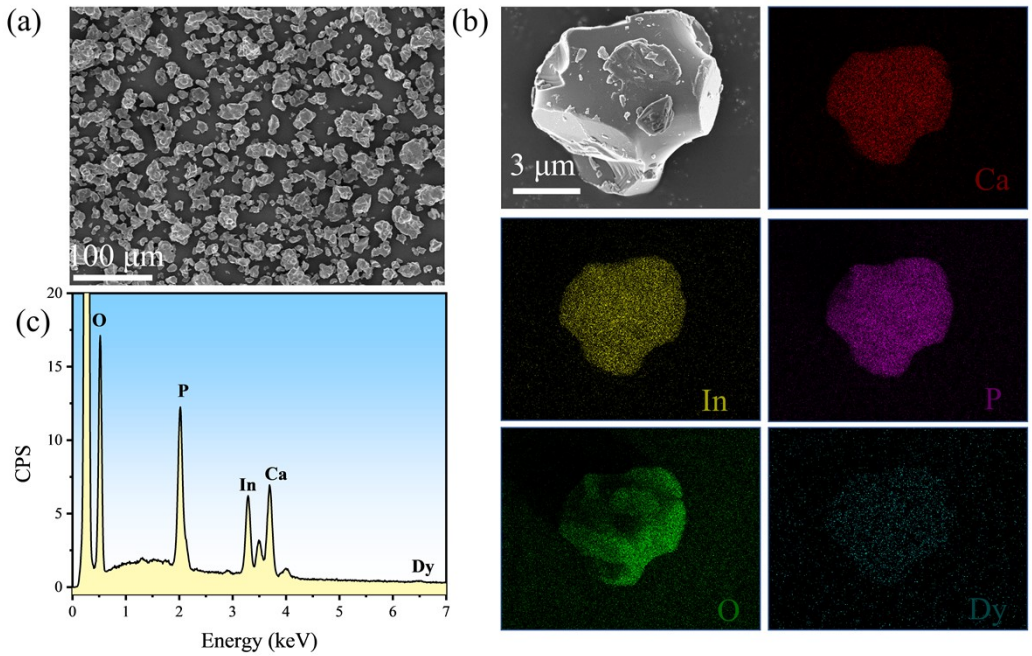

Figure S4. SEM image (a), EDS elemental mappings (b), and EDS spectrum (c) of $C_{1-x}IP$: $0.03Dy^{3+}$ sample.

Table S7. The result of XPS analysis for $C_{1-x}IP$: $0.03Dy^{3+}$.

Element	Ca	In	P	O	Dy
Theory (at%)	10.12	8.70	16.35	64.52	0.31
XPS Value (at%)	8.49	6.79	17.66	66.86	0.20

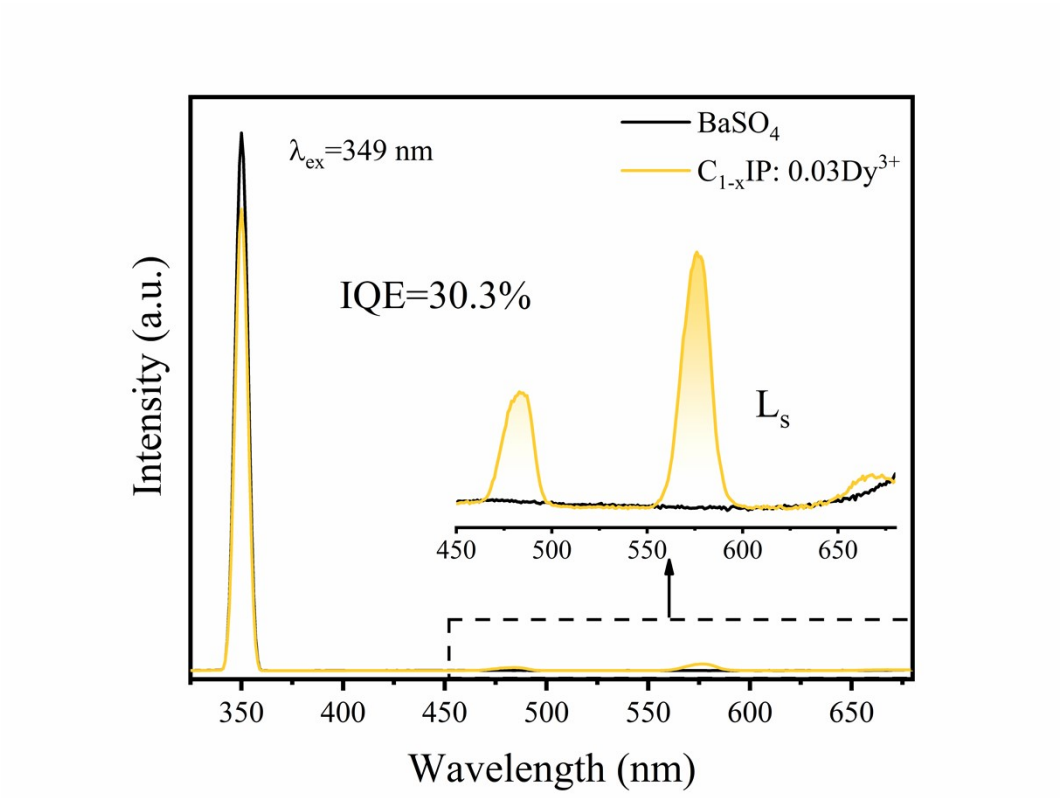

Figure S5. Excitation line of $BaSO_4$ and emission spectrum for $C_{1-x}IP$:$0.03Dy^{3+}$ phosphor.