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Supplementary Information

Site-Selective Cation Distribution and Structural Distortion in $Y_3Al_{5-x}Ga_xO_{12}$:Pr Garnet Phosphors: A Multi-Analytical Investigation

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Table S1. *Rietveld refinement data of $Y_3Al_{5-x}Ga_xO_{12}$ (x = 0, 1, 2, 2.5, 3, 3.5, 4, 5).*

x	0	1	2	2.5	3	3.5	4	5
Radiation type; λ (Å)	X-ray; 1.5406	X-ray; 1.5406	X-ray; 1.5406	X-ray; 1.5406	X-ray; 1.5406	X-ray; 1.5406	X-ray; 1.5406	X-ray; 1.5406
2θ (degree)	10 - 80	10 - 80	10 - 80	10 - 80	10 - 80	10 - 80	10 - 80	10 - 80
Temperature (K)	298	298	298	298	298	298	298	298
Space group	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$
α = β = γ (degree)	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
a = b = c (Å)	12.0075	12.0601	12.1106	12.1454	12.15273	12.21162	12.2309	12.2861
V (Å^3)	1 731.2420	1 754.0934	1 776.2209	1 791.5769	1 794.8226	1 821.0325	1 829.6804	1 854.5653
Profile R-factor, R_p	0.0381	0.04216	0.04732	0.0520	0.4342	0.4672	0.0449	0.4821
Weighted profile R-factor, R_{wp}	0.0723	0.07821	0.07425	0.0758	0.0850	0.0893	0.0857	0.08145

Table S2. *Atomic positions and occupancies derived for $Y_3Al_{5-x}Ga_xO_{12}$ (x = 0, 1, 2, 2.5, 3, 3.5, 4, 5) determined through the Rietveld refinement of XRD data.*

x = 0

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24c	1	0.2500	0.12500	0	0.00187
Al(1)	16a	1	0	0	0	0.00187
Al(2)	24d	1	0.25000	0.375000	0	0.00322
O(1)	96h	1	0.031280	0.049598	0.150	0.01163

x=1

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24c	1	0.2500	0.12500	0	0.00987
Al(1)	16a	0.8918	0	0	0	0.00563
Al(2)	24d	0.7270	0.25000	0.375000	0	0.00923
Ga (1)	16a	0.1082	0	0	0	0.00748
Ga (2)	24d	0.2730	0.25000	0.375000	0	0.00686
O(1)	96h	1	0.030248	0.052281	0.65306	0.01163

x= 2

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24c	1	0.2500	0.12500	0	0.00982
Al(1)	16a	0.7084	0	0	0	0.00486
Al(2)	24d	0.4693	0.25000	0.375000	0	0.01970
Ga (1)	16a	0.2916	0	0	0	0.06208
Ga (2)	24d	0.5307	0.25000	0.375000	0	0.00256
O(1)	96h	1	0.032378	0.058005	0.624921	0.002401

x= 2.5

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24*c*	1	0.1250	0	0.2500	0.00865
Al(1)	16*a*	0.6437	0	0	0	0.03832
Al(2)	24*d*	0.4281	0.37500	0	0.2500	0.01970
Ga (1)	16*a*	0.3563	0	0	0	0.007000
Ga (2)	24*d*	0.5719	0.37500	0	0.2500	0.00509
O(1)	96*h*	1	0.037061	0.041259	0.634075	0.01042

x= 3

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24*c*	1	0.1250	0	0.2500	0.00263
Al(1)	16*a*	0.5455	0	0	0	0.00501
Al(2)	24*d*	0.3412	0.37500	0	0.2500	0.01612
Ga (1)	16*a*	0.4545	0	0	0	0.00254
Ga (2)	24*d*	0.6579	0.37500	0	0.2500	0.00221
O(1)	96*h*	1	0.0365321	0.0431899	0.644015	0.01042

x= 3.5

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24*c*	1	0.1250	0	0.2500	0.02672
Al(1)	16*a*	0.4548	0	0	0	0.00305
Al(2)	24*d*	0.2391	0.37500	0	0.2500	0.00263
Ga (1)	16*a*	0.5252	0	0	0	0.00803
Ga (2)	24*d*	0.7609	0.37500	0	0.2500	0.00409
O(1)	96*h*	1	-0.027200	0.055800	0.15000	0.00813

x= 4

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24*c*	1	0.1250	0	0.2500	0.0830
Al(1)	16*a*	0.2708	0	0	0	0.00930
Al(2)	24*d*	0.1978	0.37500	0	0.2500	0.00812
Ga (1)	16*a*	0.7292	0	0	0	0.00933
Ga (2)	24*d*	0.8022	0.37500	0	0.2500	0.00233
O(1)	96*h*	1	-0.02578	0.05523	0.152430	0.002515

x= 5

Atom	Wyck. position	Occupation	*x*	*y*	*z*	U_{iso}
Y(1)	24*c*	1	0.1250	0	0.2500	0.00436
Ga (1)	16*a*	0.7292	0	0	0	0.00620
Ga (2)	24*d*	0.8022	0.37500	0	0.2500	0.01072
O(1)	96*h*	1	-0.02857	0.055369	0.150089	0.00809

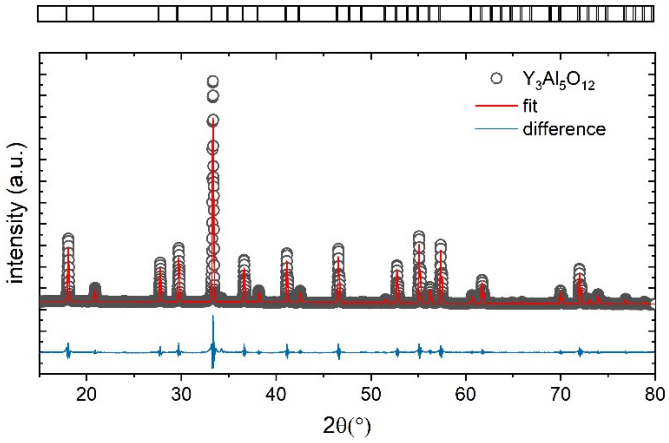

Figure S1*. Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3Al_5O_{12}$:Pr.*

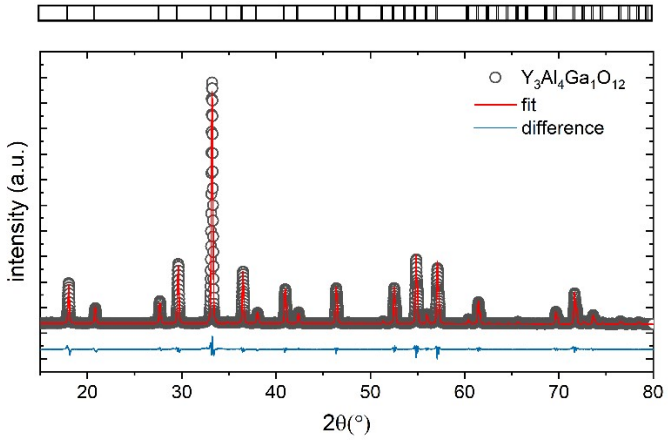

Figure S2. *Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3(Al_4Ga_1)O_{12}$:Pr.*

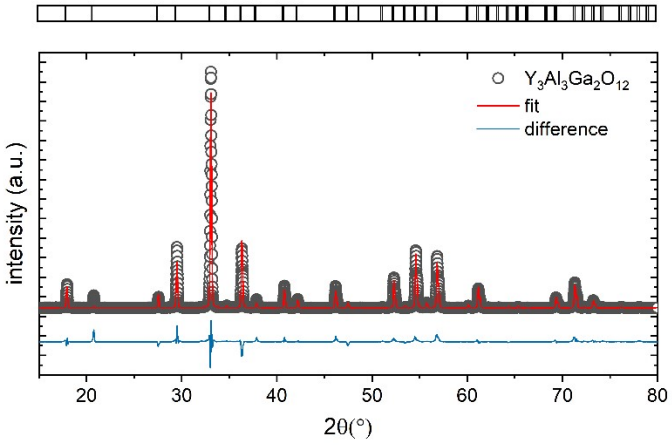

Figure S3*. Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3(Al_3Ga_2)O_{12}$:Pr.*

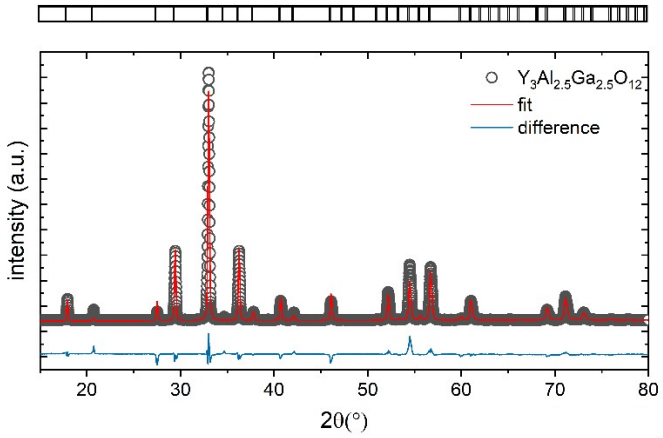

***Figure S4**. Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3(Al_{2.5}Ga_{2.5})O_{12}$:Pr.*

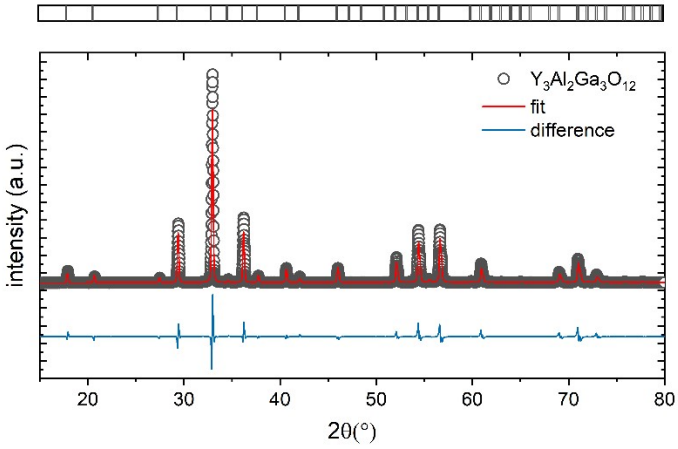

***Figure S5**. Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3(Al_2Ga_3)O_{12}$:Pr.*

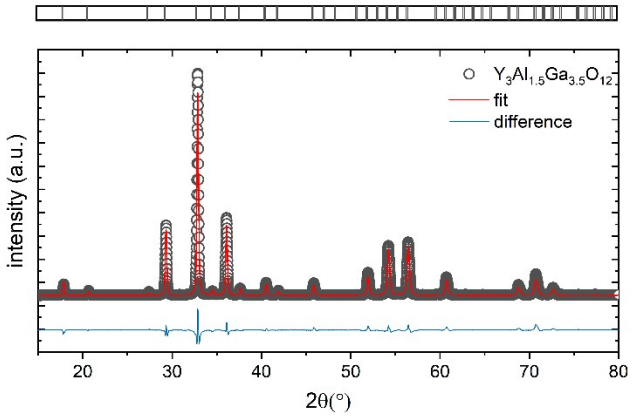

Figure S6. *Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3(Al_{1.5}Ga_{3.5})O_{12}$:Pr.*

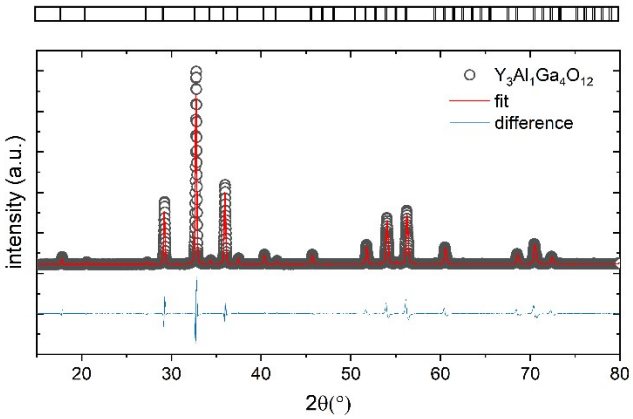

Figure S7*. Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3(Al_1Ga_4)O_{12}$:Pr.*

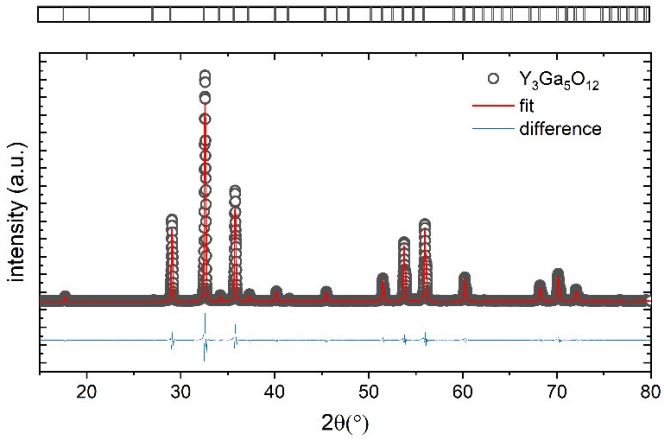

***Figure S8**. Measured XRD diffractograms (black), the Rietveld fit (red), and the difference between them (blue) for $Y_3Ga_5O_{12}$:Pr.*

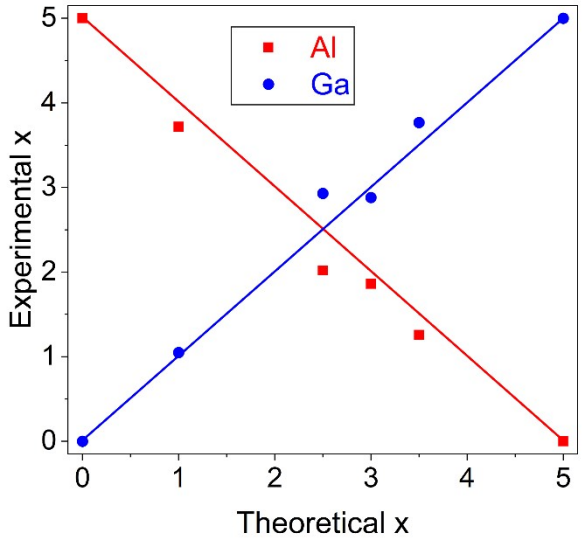

***Figure S9**. Experimental vs. theoretical x-value in $Y_3Al_{5-x}Ga_xO_{12}$:Pr calculated based on the XRF analysis.*