

Supporting Materials

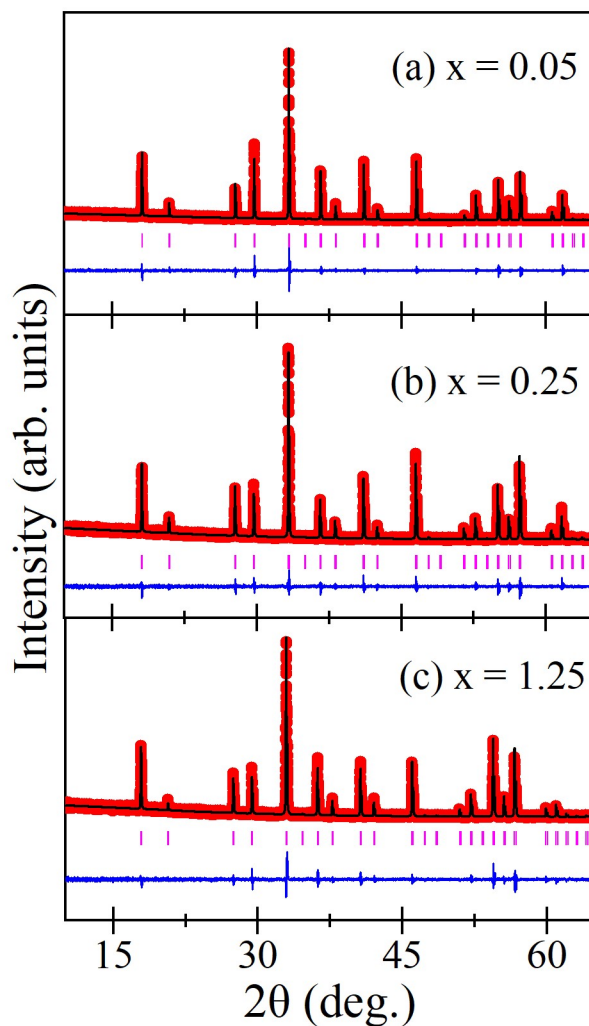


Figure S1. Observed (red circle), calculated (black line) and difference (blue line) profiles obtained from Rietveld refinement of $\text{Y}_3\text{Al}_{5-x}\text{Sc}_x\text{O}_{12}$ garnet: (a) $x = 0.05$, (b) $x = 0.25$, and (c) $x = 1.25$ using $Ia-3d$ space group. The vertical line (pink) indicates the Bragg peak positions.

Table S1. Crystallographic parameters obtained from Rietveld refinement for different compositions of $\text{Y}_3\text{Al}_{5-x}\text{Sc}_x\text{O}_{12}$ garnet.

Y ₃ Al _{5-x} Sc _x O ₁₂	x = 0.05	x = 0.25	x = 1.25
Crystal Structure	Cubic		
Unit Cell	Ia-3d		
Lattice Constant			
a = b = c (Å)	12.0138(7)	12.0263(9)	12.1454(5)
V (Å) ³	1733.98(8)	1739.40(4)	1791.57(5)
Atomic Coordinates			
Y ³⁺ 24c			
x	0.1250	0.1250	0.1250
y	0.0000	0.0000	0.0000
z	0.2500	0.2500	0.2500
Al ³⁺ /Sc ³⁺ 16a			
x	0.0000	0.0000	0.0000
y	0.0000	0.0000	0.0000
z	0.0000	0.0000	0.0000
Al ³⁺ /Sc ³⁺ 24d			
x	0.3750	0.3750	0.3750
y	0.0000	0.0000	0.0000
z	0.2500	0.2500	0.2500
O ²⁻ 96h			
x	0.1810	0.3130	0.2481
y	0.0522	0.0584	0.0543
z	0.0474	0.0497	0.0482

Bond Distance			
Y ₁ -O ₁ (Å)	2.312	2.321	2.426
Al/Sc ₁ -O ₁ (Å)	1.941	1.943	1.992
Y ₁ -Al/Sc ₁ (Å)	3.359	3.362	3.393
Y ₁ -Y ₁ (Å)	3.680	3.683	3.723
Goodness of refinement fit			
χ^2	1.40	1.23	2.82