Table S1. Initial data for full-profile analysis using HighScore Plus v.3.0.5 software.

Cation	Wyckoff	Coordinates			Sof (AP-01)	Sof (AP-02)	Sof (AP-03)
		x	y	z			
Y^{3+}_{C}	24c	0.125	0	0.25	0.78	0.5533	0.32
Yb^{3+}_{C}	24c	0.125	0	0.25	0.15	0.15	0.15
Er^{3+}_{C}	24c	0.125	0	0.25	0.03	0.03	0.03
Sc^{3+}_{C}	24c	0.125	0	0.25	0.04	0.2667	0.5
Sc^{3+}_{A}	16a	0	0	0	0.04	0.1	0.1
Al^{3+}_{A}	16a	0	0	0	0.96	0.9	0.9
Al^{3+}_{D}	24d	0.375	0	0.25	1	1	1
O^{2-}_{O}	96h	-0.032	0.051	0.150	1	1	1

Table S2 Refined structural and electronic properties of samples

Sample		AP-1	AP-2	AP-3
space group		Ia-3d	Ia-3d	Ia-3d
(a_G), Å		12.00441(6)	11.95139(5)	11.87350(6)
Coordinates	X (96h)	-0.03009	-0.02931	-0.02863
	y(96h)	0.051	0.05265	0.05281
	z(96h)	0.1495	0.15092	0.15115

Table S3. Agreement Indices

Agreement Indices		AP-01	AP-02	AP-03
	R expected	1.759	1.88	2.10922
	R profile	2.947	3.581	3.00029
	Weighted R profile	3.892	5.606	4.0155
	D-statistics	0.422	0.39	0.47779
	Weighted D-statistics	0.374	0.203	0.42526
	Goodness of Fit	4.893	8.888	3.6244
	R Bragg	4.07	6.61	4.53