Supporting Information

K^+-Doped P$\bar{6}$ Crystals of NIR-Upconverting $NaYF_4$:Yb^{3+}/Ho^{3+} conforms to the 'Strain-Intensity' Relationship

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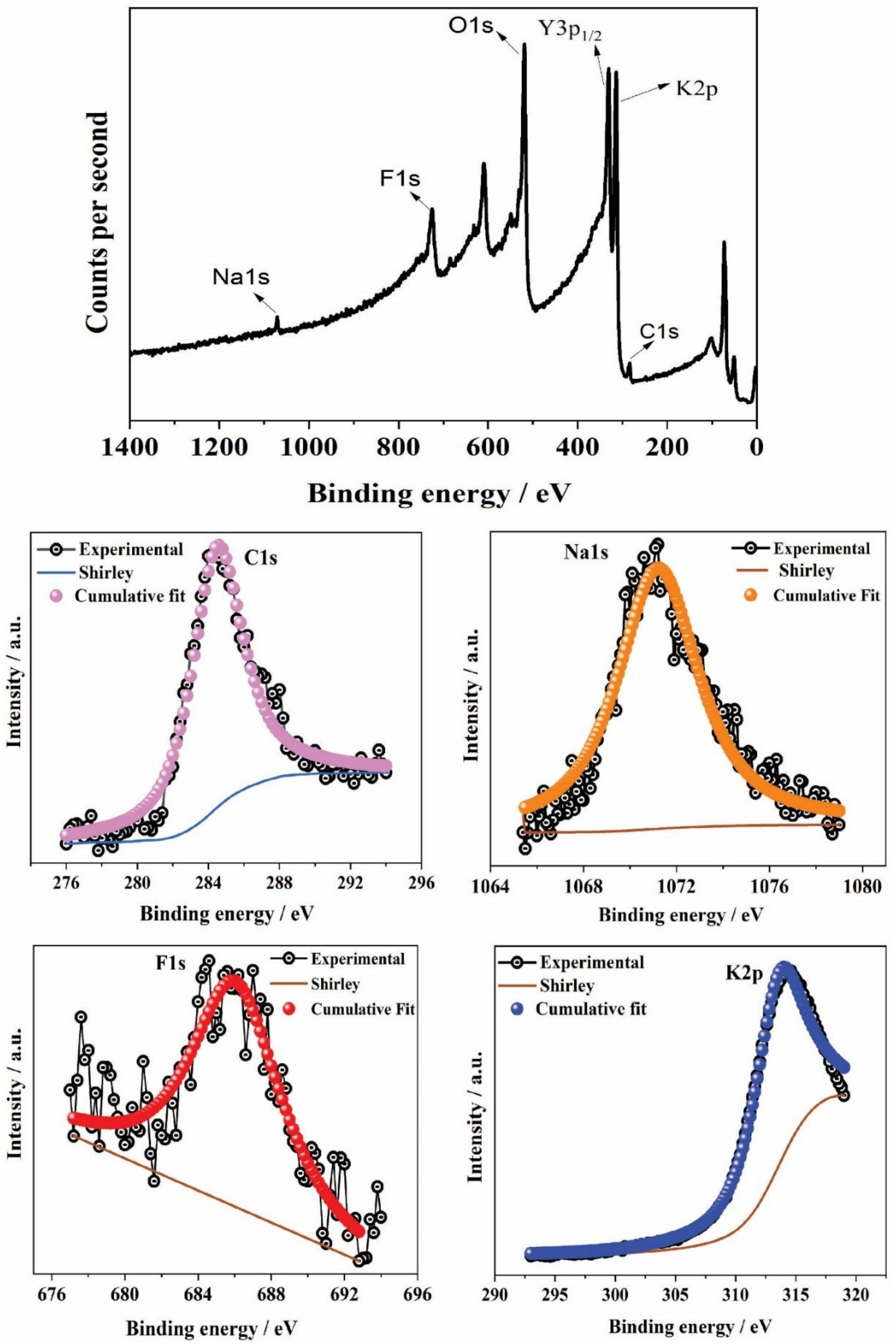


Figure S1. XPS spectrum of oleic acid capped sample K1 synthesized by thermal decomposition method and cumulative peak fit.

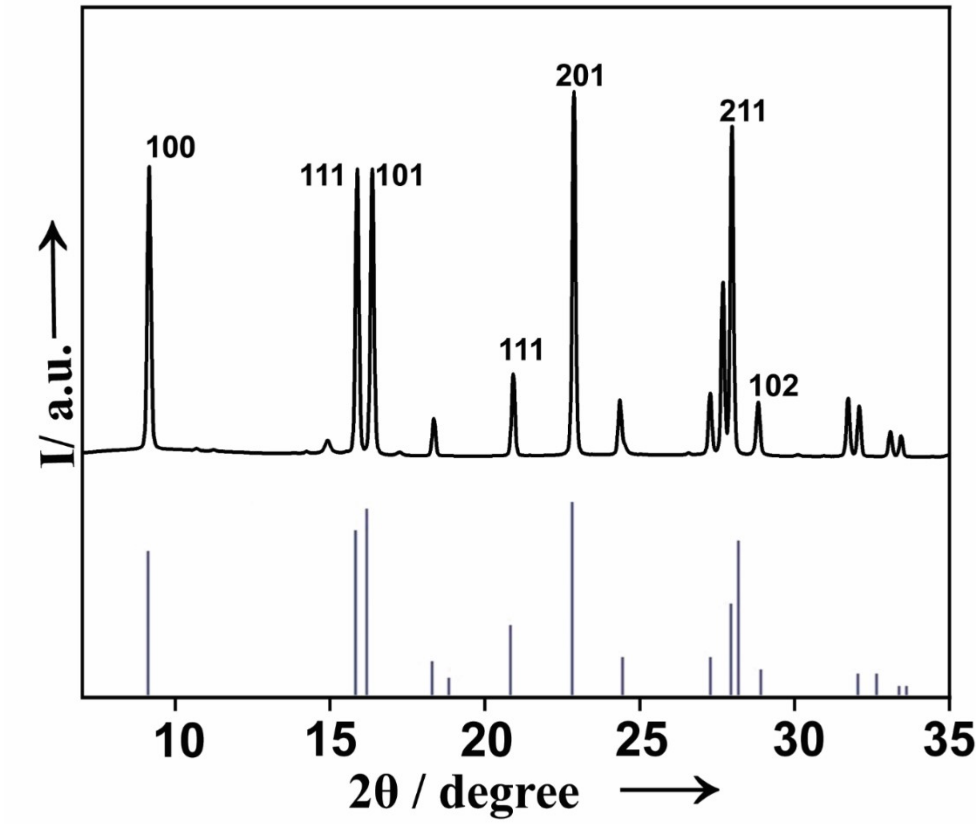


Figure S2: XRD pattern of as synthesized β-$NaYF_4$:Yb^{3+}/Ho^{3+} matching with the standard diffraction pattern of β-$NaYF_4$ (JCPDS No-16-0334).

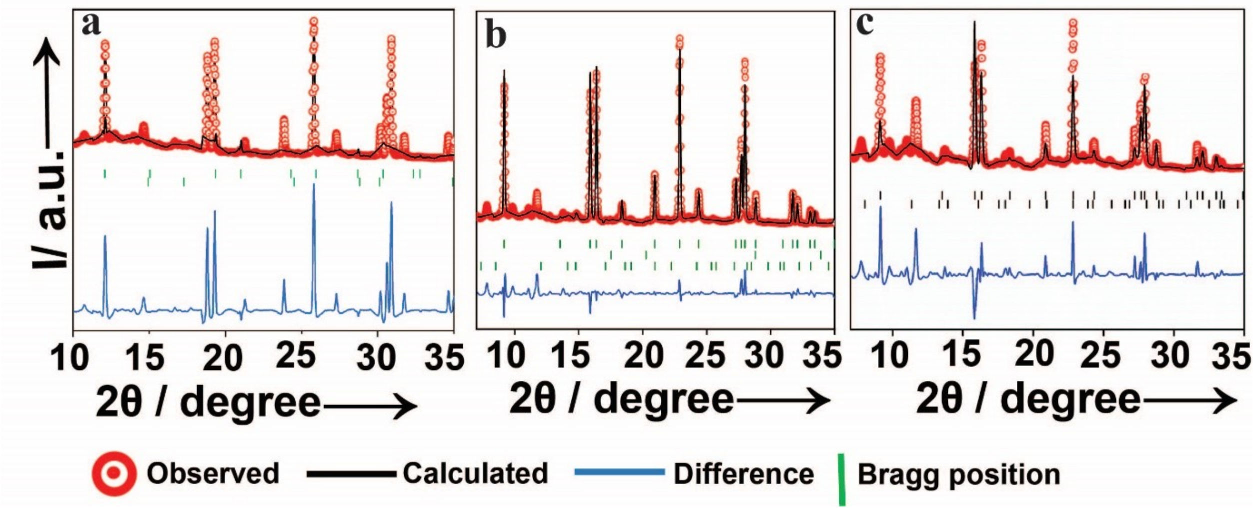


Figure S3: Rietveld refinement plots of ADXRD data of (a) K6 (b) K7 and (c) K8.

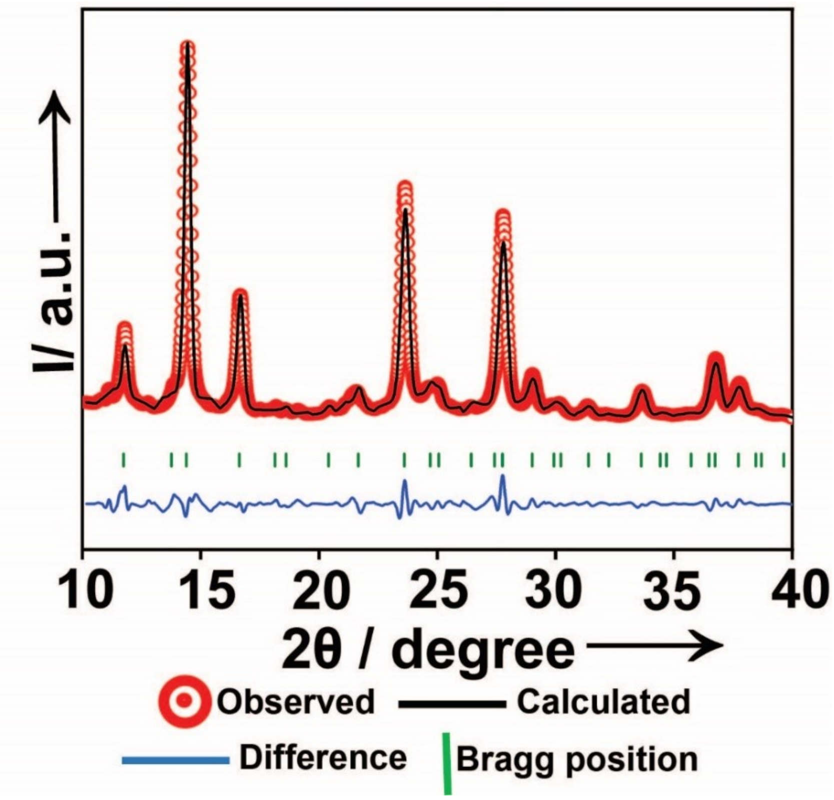


Figure S4: Rietveld refinement plot of cubic KYb_3F_{10} (K48).

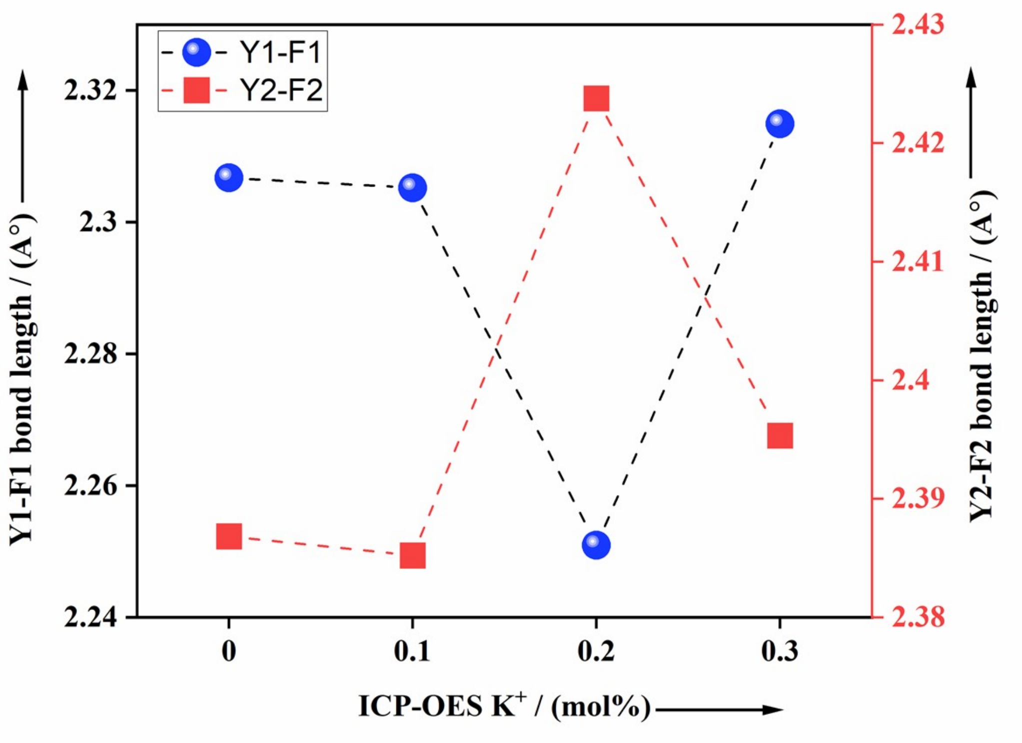


Figure S5: Y1-F1 and Y2-F2 bond lengths obtained from Rietveld refinement analysis of samples K0, K1, K2 and K3.

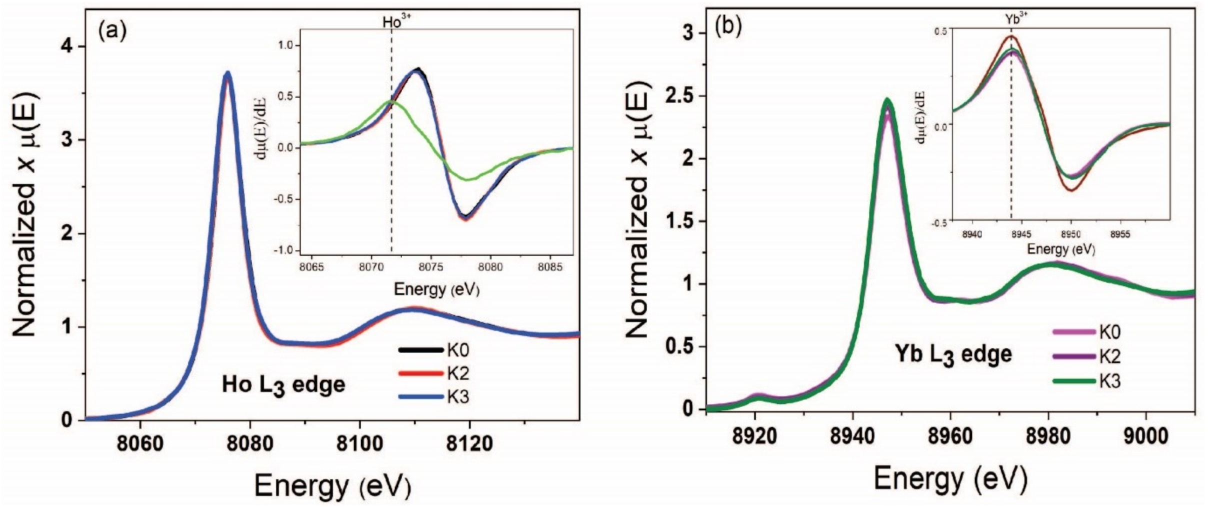


Figure S6. The normalized XANES spectra of samples K0, K2 and K3 at (a) Ho L_3 edge and (b) Yb L_3 edge. The inset shows the 1st derivative along with the reference's oxide (+3 state).

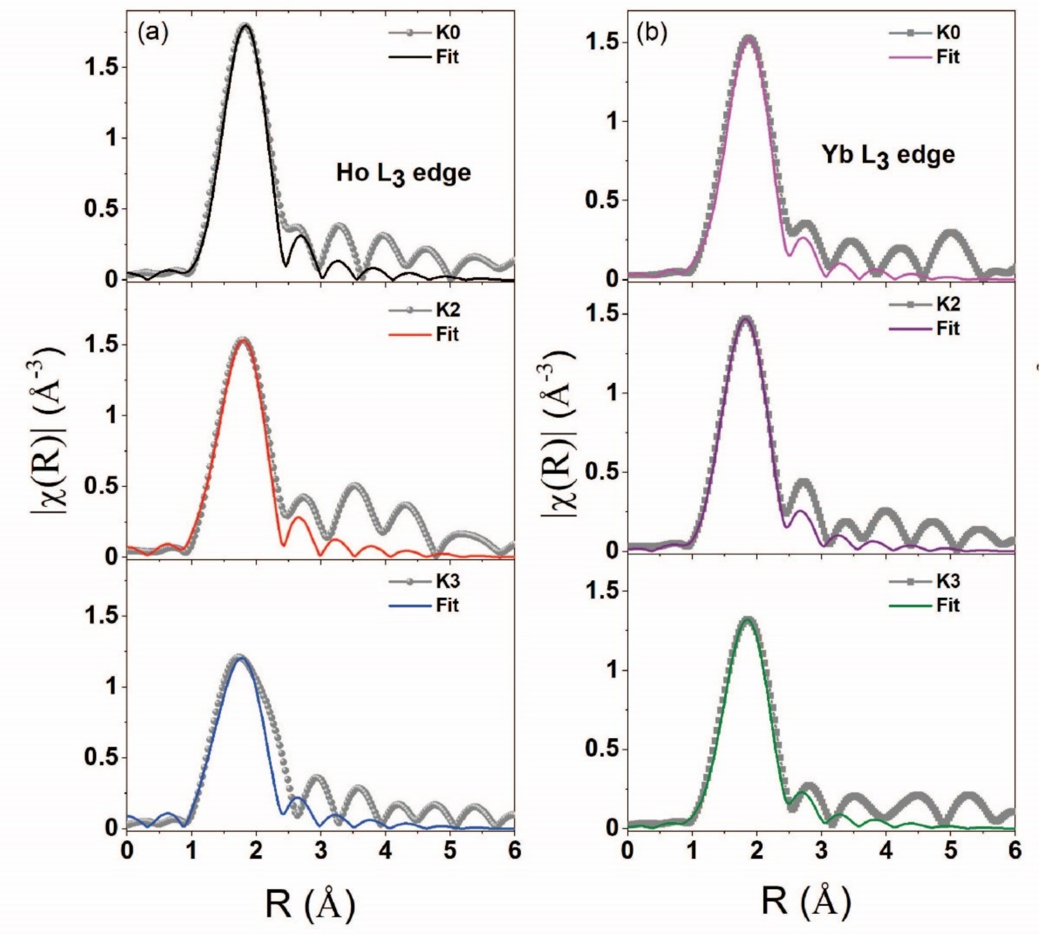


Figure S7. The Fourier Transform (FT) of k^2-weighted $\chi(k)$ spectra of K0, K2 and K3 at (a) Ho L_3 edge and, (b) Yb L_3 edges, respectively.

Table S1. Shows the variation of CN (coordination number), R (bond distance) and σ^2 (DebyeWaller factor) by EXAFS data fitting at Ho L_3-edge, Y K-edge and Yb L_3-edge. The numbers in parentheses indicate the uncertainty in the last digit.

	Ho L_3-edge			Y K-edge			Yb L_3-edge		
Sample	CN_{Ho-F}	R_{Ho-F}(Å)	σ^2_{Ho-F}(Å^2)	CN_{Y-F}	R_{Y-F}(Å)	σ^2_{Y-F} (Å^2)	CN_{Yb-F}	R_{Yb-F} (Å)	σ^2_{Yb-F} (Å^2)
K-0	8.6 (2)	2.274 (2)	0.0032 (3)	7.2 (2)	2.379 (3)	0.0091 (3)	8.2 (2)	2.277 (2)	0.0064 (3)
K-20	7.8 (2)	2.235 (3)	0.0046 (3)	7.4 (2)	2.293 (2)	0.0085 (3)	8.1 (2)	2.249 (3)	0.0064 (3)
K-30	7.4 (2)	2.232 (3)	0.0072 (3)	7.5 (2)	2.211 (2)	0.0088 (3)	7.8 (2)	2.271 (3)	0.0076 (3)

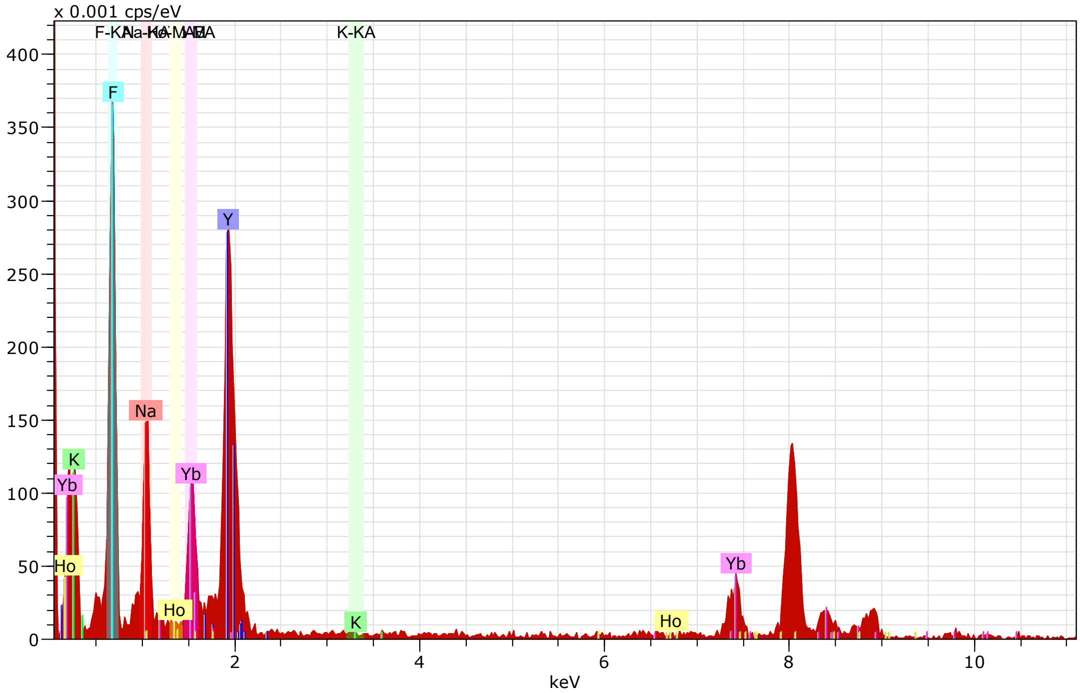


Figure S8: EDS spectra of sample K1.

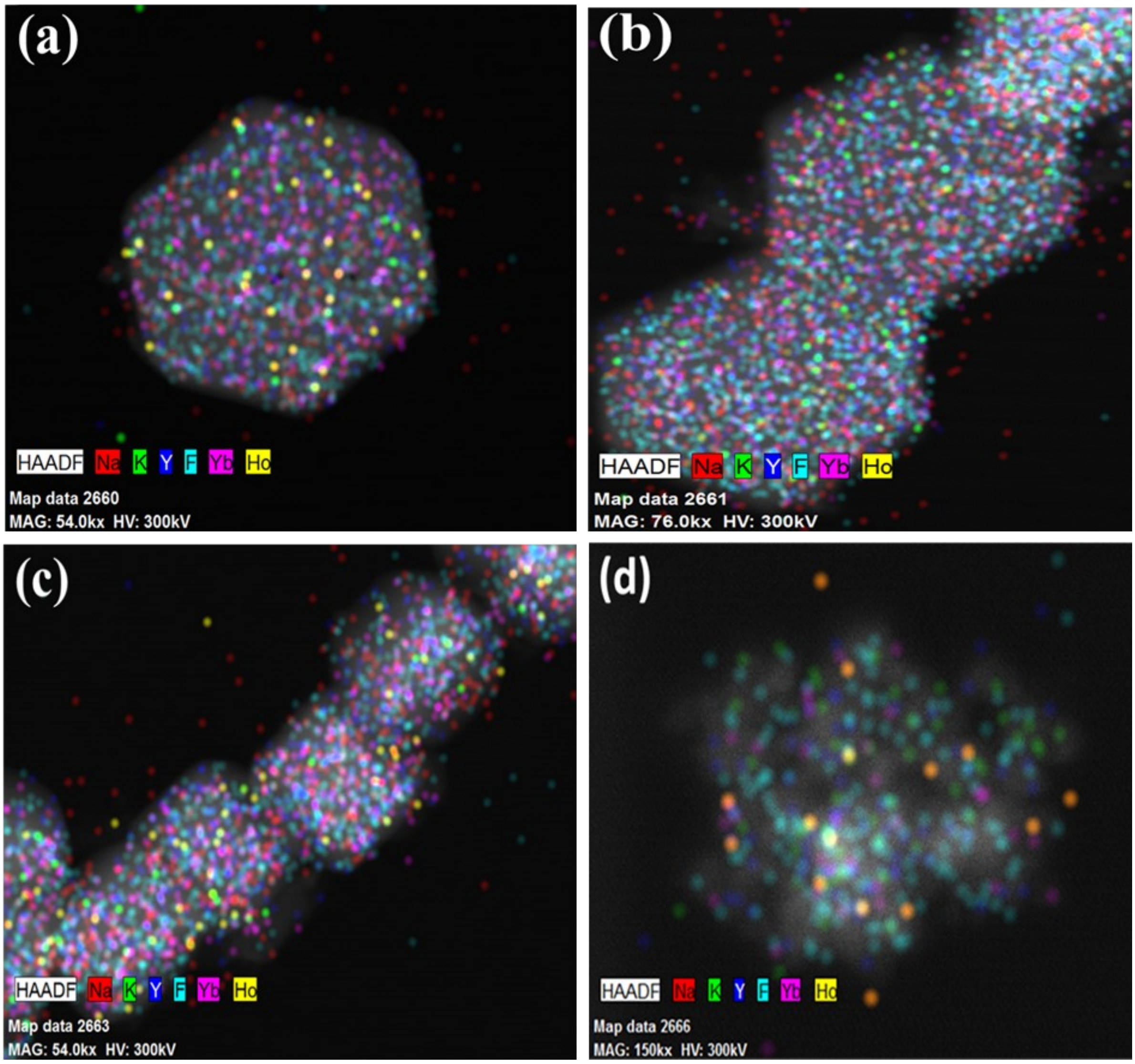


Figure S9: EDS-based elemental mapping of sample (a) K1, (b) K2, (c) K3, (d) K48

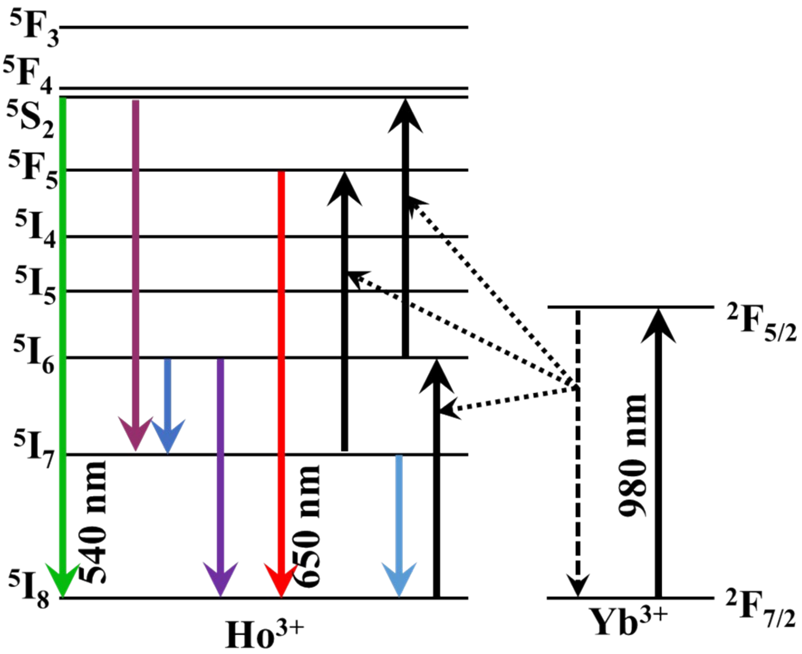
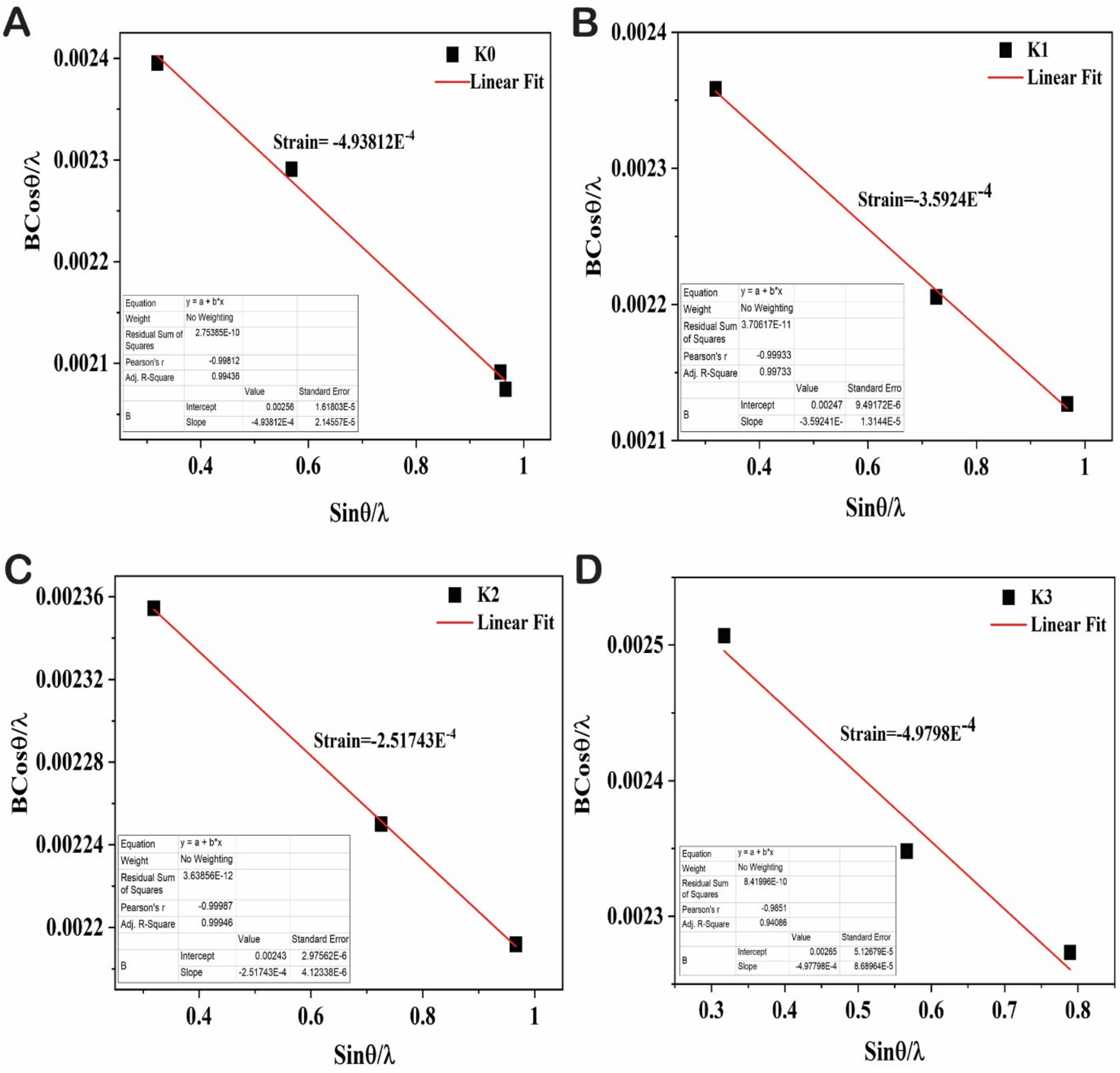


Figure S10: Schematic of energy-level diagram of upconversion luminescence in $NaYF_4$:Yb^{3+}/Ho^{3+} involving Yb^{3+} (sensitiser) and Ho^{3+} (activator), and the proposed mechanism of upconversion luminescence.



Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	2.75385E-10		
Pearson's r	-0.99812		
Adj. R-Square	0.99436		
		Value	Standard Error
B	Intercept	0.00256	1.61803E-5
	Slope	-4.93812E-4	2.14557E-5

Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	3.70617E-11		
Pearson's r	-0.99933		
Adj. R-Square	0.99733		
		Value	Standard Erro
B	Intercept	0.00247	9.49172E-6
	Slope	-3.59241E-	1.3144E-5

Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	3.63856E-12		
Pearson's r	-0.99987		
Adj. R-Square	0.99946		
		Value	Standard Error
B	Intercept	0.00243	2.97562E-6
	Slope	-2.51743E-4	4.12338E-6

Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	8.41996E-10		
Pearson's r	-0.9851		
Adj. R-Square	0.94086		
		Value	Standard Error
B	Intercept	0.00265	5.12679E-5
	Slope	-4.97798E-4	8.68964E-5

Figure S11: Williamson-Hall plots of samples K0 to K3 UC crystals. Strain is obtained from the slope of the fit.

Lattice strain calculation using Williamson hall Plot

The micro strain present in the lattice of materials were calculated by Williamson Hall (W-H) plot governed by the mathematical equation:

$$\frac{\beta\, cos\theta}{\lambda} = \frac{1}{D} + \frac{\varepsilon\, Sin\theta}{\lambda}$$

Where, λ is the wavelength of radiation (x-ray from synchrotron radiation= 0.75428 Å), β is full width at half maximum (FWHM) of diffraction peak, D is the crystallite size in Å, θ is the peak position and ε is the micro strain present in the sample. Plots are drawn between sinθ/λ and βcosθ/λ and micro strain is calculated from slope and particle size from intercept at Y-axis of the fit.