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Supporting Information for

Controlled Synthesis and Upconversion Luminescence of Lanthanide Doped BaYF₅ Nanocrystals

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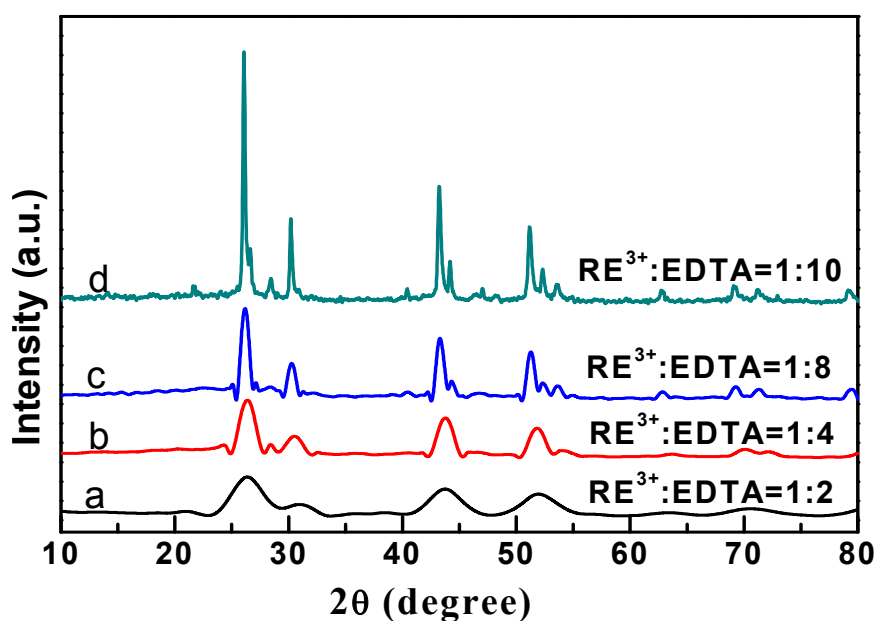


Figure S1. The typical XRD patterns of BaYF₅ with the RE³⁺/EDTA of (a)1:2, (b)1:4, (c)1:8, and (d)1:10, respectively.

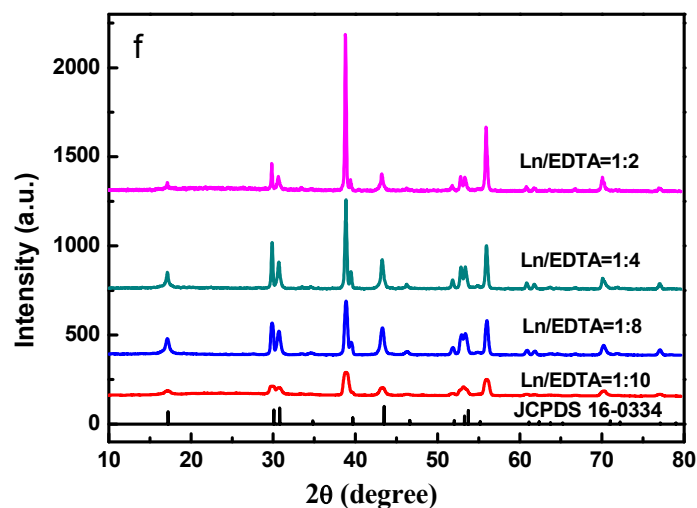
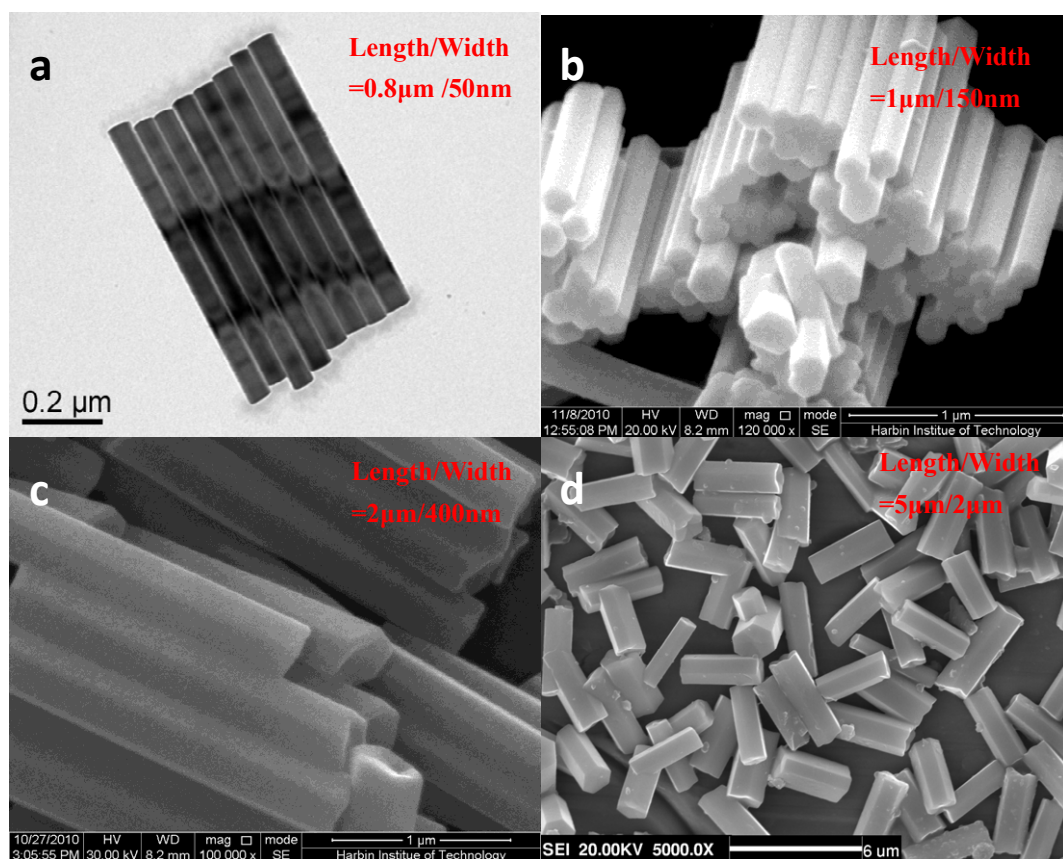


Figure S2. (a) TEM, (b, c and d) FESEM images of NaYF₄ with the RE³⁺/EDTA of (a)1:10, (b)1:8, (c)1:4, and (d)1:2, respectively. (f) XRD patterns of NaYF₄ powders in Figure S2 (a-d). All the diffraction peaks of NaYF₄ powders with RE³⁺/EDTA of (a)1:10, (b)1:8, (c)1:4, and (d)1:2 agree well with standard hexagonal structure of JCPDS 16-0334.

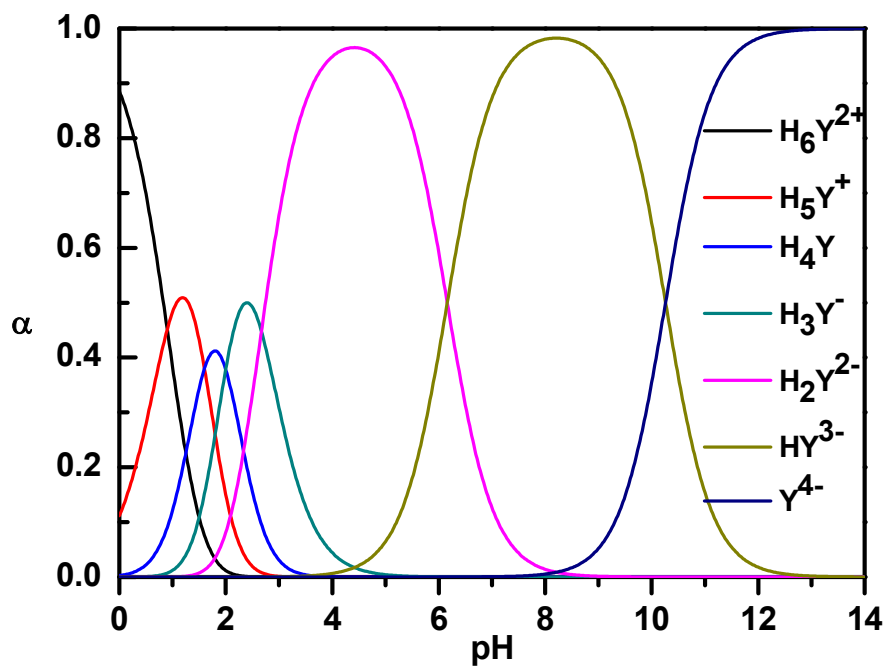


Figure S3. Relative distribution of species of EDTA versus the pH value.

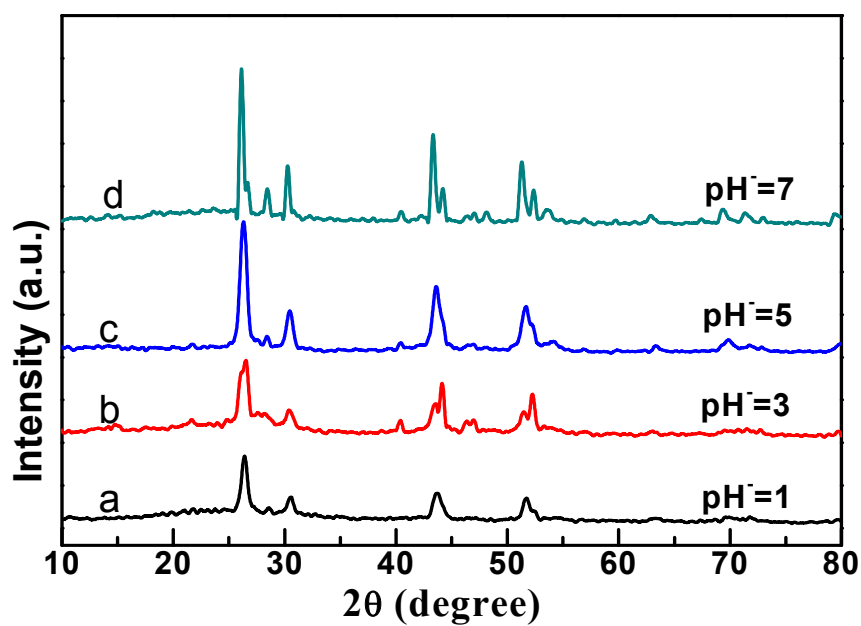


Figure S4. The typical XRD patterns of BaYF₅ at (a) pH=1, (b)pH=3, (c) pH=5, and (d) pH=7, respectively

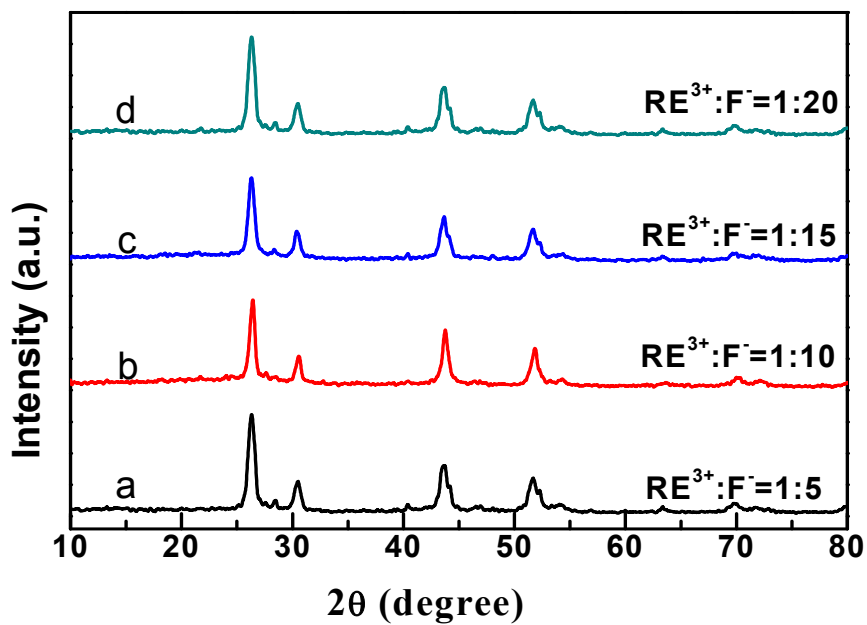


Figure S5. The typical XRD patterns of BaYF₅ with RE³⁺/F⁻ ratio of (a) 1:5 (b) 1:10, (c) 1:15 and (d) 1:20, respectively.

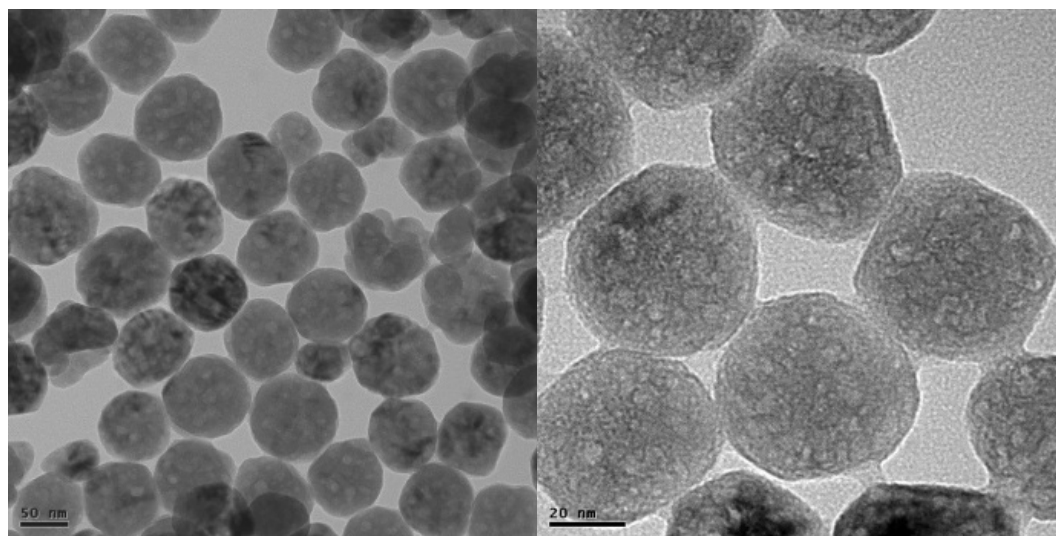


Figure S6. TEM images of BaYF₅ nanocrystals after ligand exchange.

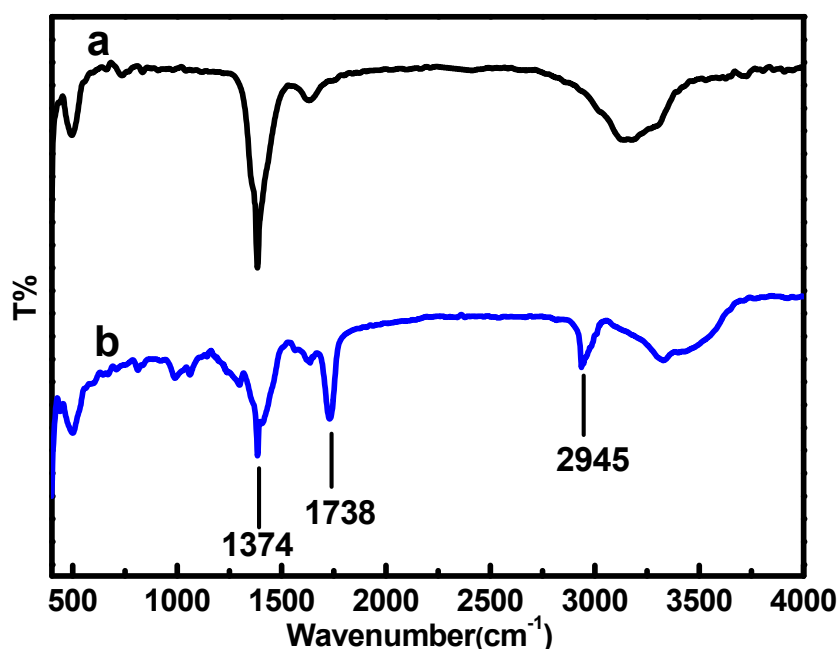


Figure S7. Fourier transform infrared (FT-IR) spectra of BaYF₅ nanocrystals before (a) and after (b) ligand exchange using PAA. Photographs of colloidal solutions of the BaYF₅ nanocrystals (50-60nm) dispersed in cyclohexane and water before (c) and after (d) PAA modification. The FT-IR spectra were used to characterize the functional groups present on the surface of nanocrystals. The band at 1374 cm⁻¹ characterizing the mode of the C=O (N-CO-OH) stretching vibration in the EDTA molecule became weaker after ligand exchange (Figure S7b), suggesting the decreased EDTA molecule on the surface of BaYF₅ nanoparticles. Moreover, the bands at 1738 cm⁻¹ and 2945 cm⁻¹ newly appeared in Figure S7b characterize the -COOH group and the stretching vibration of methylene (CH₂) in the long alkyl chain, respectively, illustrating the presence of the PAA molecule on the surface of BaYF₅ nanoparticles. These observations give a strong evidence of the successful exchange of EDTA by the ligand of PAA. The broad band between 2800 cm⁻¹ and 3600 cm⁻¹ arises from the O-H stretching vibration (COO-H).

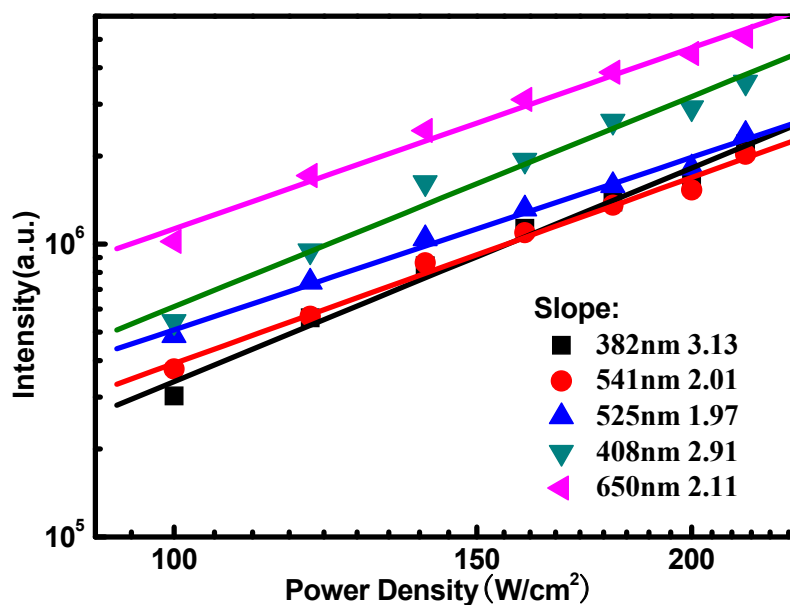


Figure S8. The dependence of the intensities of upconversion emissions bands on the power of excitation at 980 nm in the BaYF₅: 18%Yb³⁺/2%Er³⁺ system.

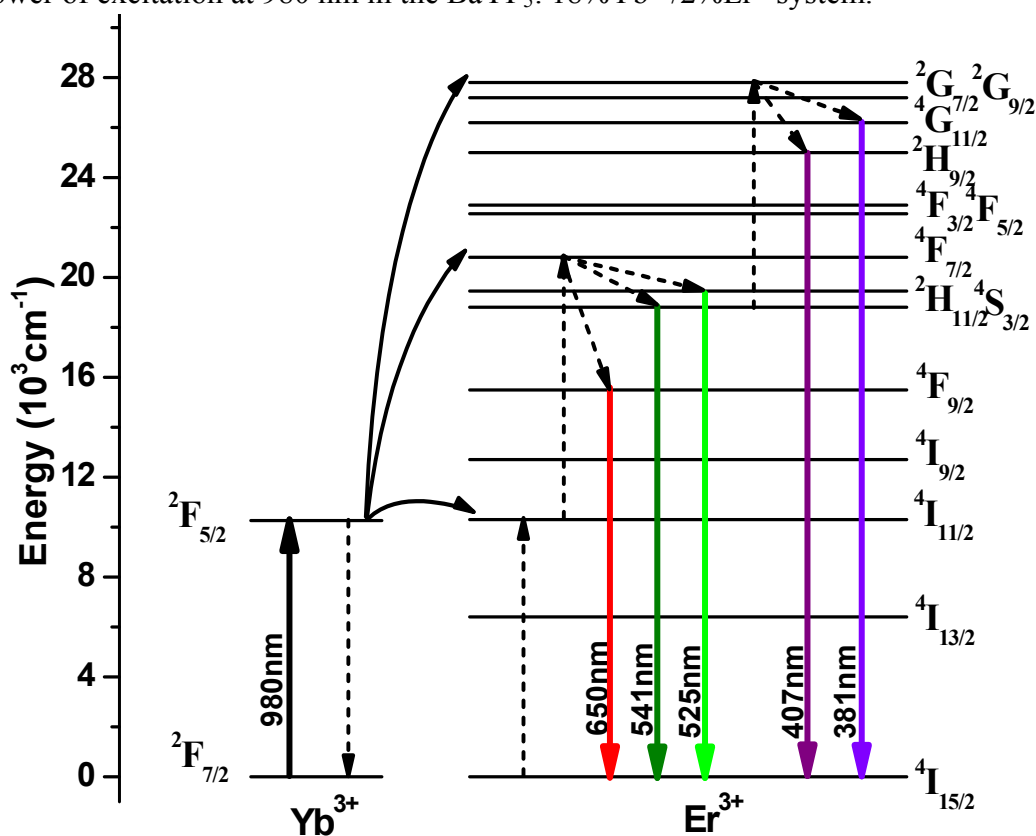


Figure S9. Schematic energy-level diagrams, upconversion excitation, and visible emission schemes for the BaYF₅: Yb³⁺/Er³⁺ system.

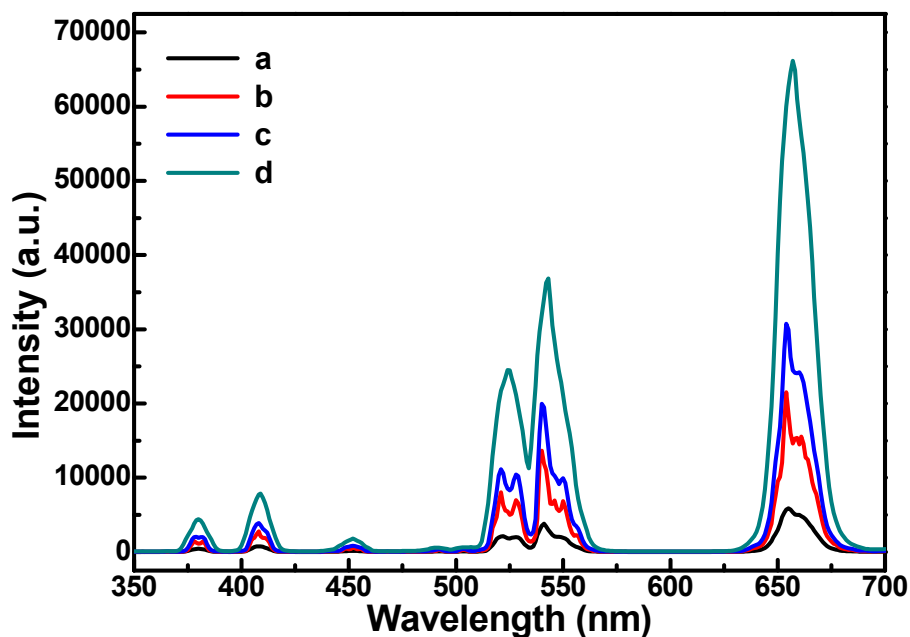


Figure S10. Upconversion emission spectra in the wavelength range of 350-700 nm of BaYF₅:18%Yb³⁺/2%Er³⁺ powders with size of (a) 10-20 nm, (b) 50-70 nm, (c) 100 nm, and (d) 1 μm microcrystals. The corresponding TEM images of BaYF₅:18%Yb³⁺/2%Er³⁺ powders with size of (a) 10-20 nm, (b) 50-70 nm, (c) 100 nm, and (d) 1 μm was shown in Figure 2.

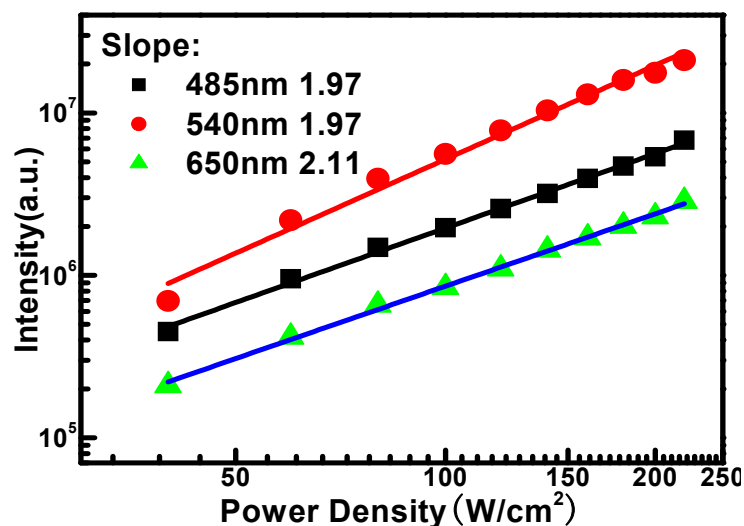


Figure S11. The dependence of the intensities of upconversion emissions bands on the power of excitation at 980 nm in the BaYF₅: 18%Yb³⁺/2%Ho³⁺ system.

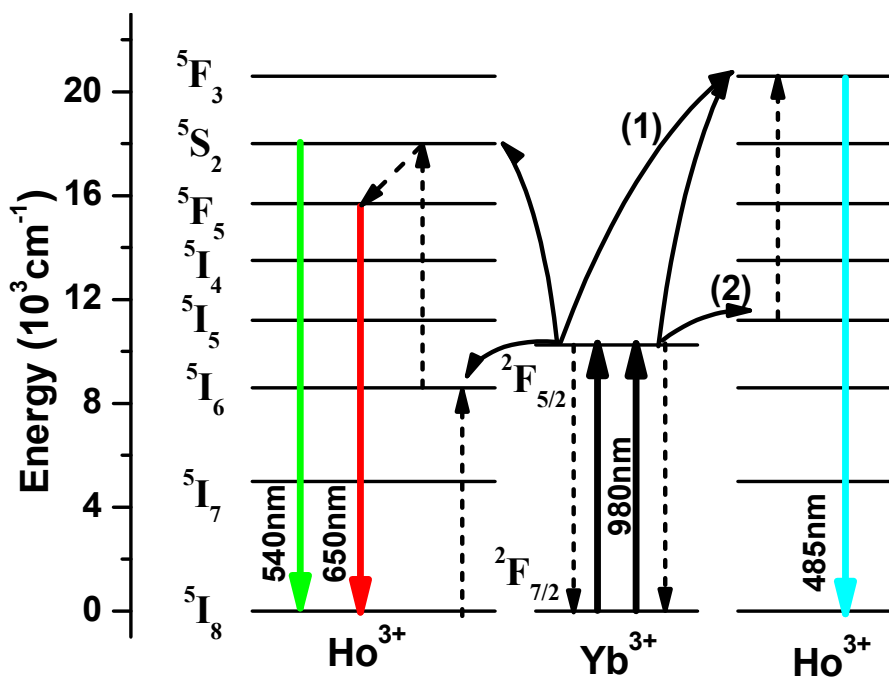


Figure S12. Schematic energy-level diagrams, upconversion excitation, and visible emission schemes for the BaYF₅: Yb³⁺/Ho³⁺ system.

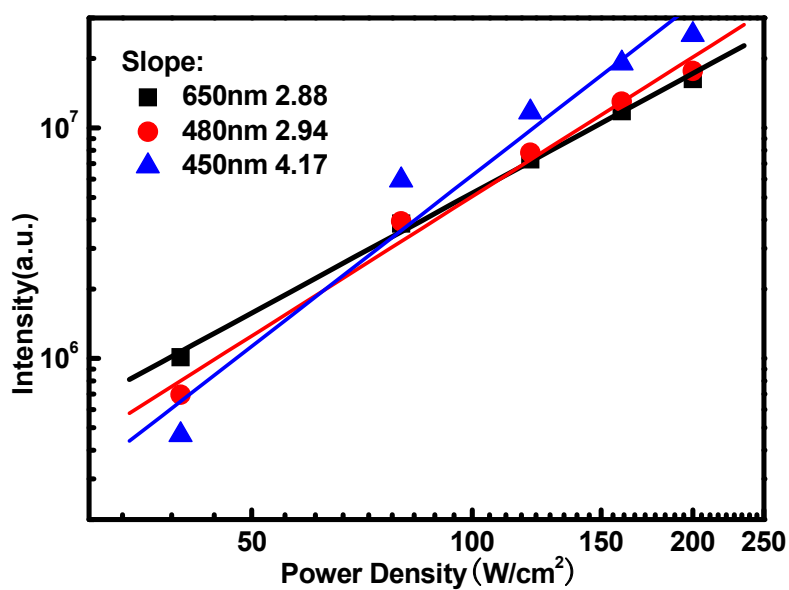


Figure S13. The dependence of the intensities of upconversion emissions bands on the power of excitation at 980 nm in the BaYF₅: 18%Yb³⁺/2%Tm³⁺ system.

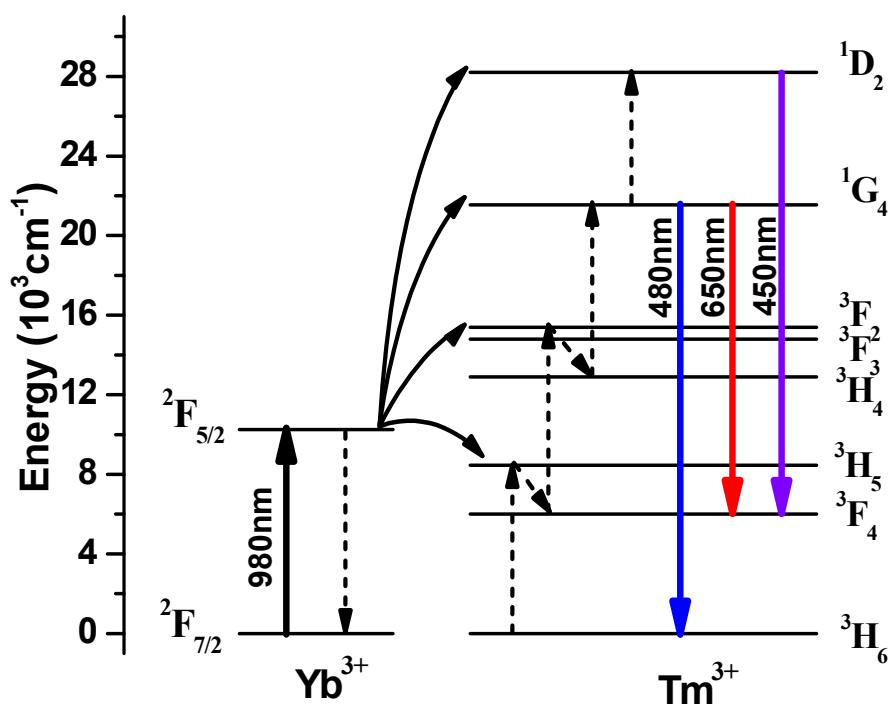


Figure S14. Schematic energy-level diagrams, upconversion excitation, and visible emission schemes for the BaYF₅: Yb³⁺/Tm³⁺ system.

Table S1. The effect of reaction conditions

Reaction conditions	Size and shape
RE ³⁺ :EDTA	
1:2	10-20nm nanoparticles
1:4	50-70 nm nanoparticles
1:8	100 nm nanoparticles
1:10	1μm cubic microcrystal
pH	
1	5-10nm nanoparticles
3	5-10nm nanoparticles
5	30-40nm nanoparticles
7	250-300nm nanoparticles
RE ³⁺ :F ⁻	
1:5	10-20nm nanoparticles
1:10	10-20nm nanoparticles
1:15	10-20nm nanoparticles
1:20	10-20nm nanoparticles