

Table S1. Crystal data and structure refinement for Li₃Ba₂Y₃(WO₄)₈ crystal.

| | |
|-----------------------------------|---|
| Empirical formula | Li ₃ Ba ₂ Y ₃ (WO ₄) ₈ |
| Formula weight | 2544.93 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, C2/c |
| Unit cell dimensions | a = 5.181(2) Å, α = 90° b = 12.677(7) Å, β = 92.237(13) ° c = 19.161(10) Å, γ = 90° |
| Volume | 1257.4(11) Å ³ |
| Z | 2 |
| Calculated density | 6.722 Mg/m ³ |
| Absorption coefficient | 46.449 mm ⁻¹ |
| F(000) | 2172 |
| Crystal size | 0.1800×0.0600×0.0500 mm |
| Theta range for data collection | 3.19 – 27.48° |
| Limiting indices | -6≤h≤6, -16≤k≤16, -24≤l≤24 |
| Reflections collected / unique | 5255 / 1439 [R(int) = 0.1660] |
| Completeness to θ = 27.48 | 99.5 % |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 1439 / 6 / 111 |
| Goodness-of-fit on F ² | 1.054 |
| Final R indices [I > 2σ(I)] | R1 = 0.0463, wR2 = 0.0976 |
| R indices (all data) | R1 = 0.0523, wR2 = 0.1009 |
| Extinction coefficient | 0.00795(12) |
| Largest diff. peak and hole | 3.574 and -4.504 e.Å ⁻³ |

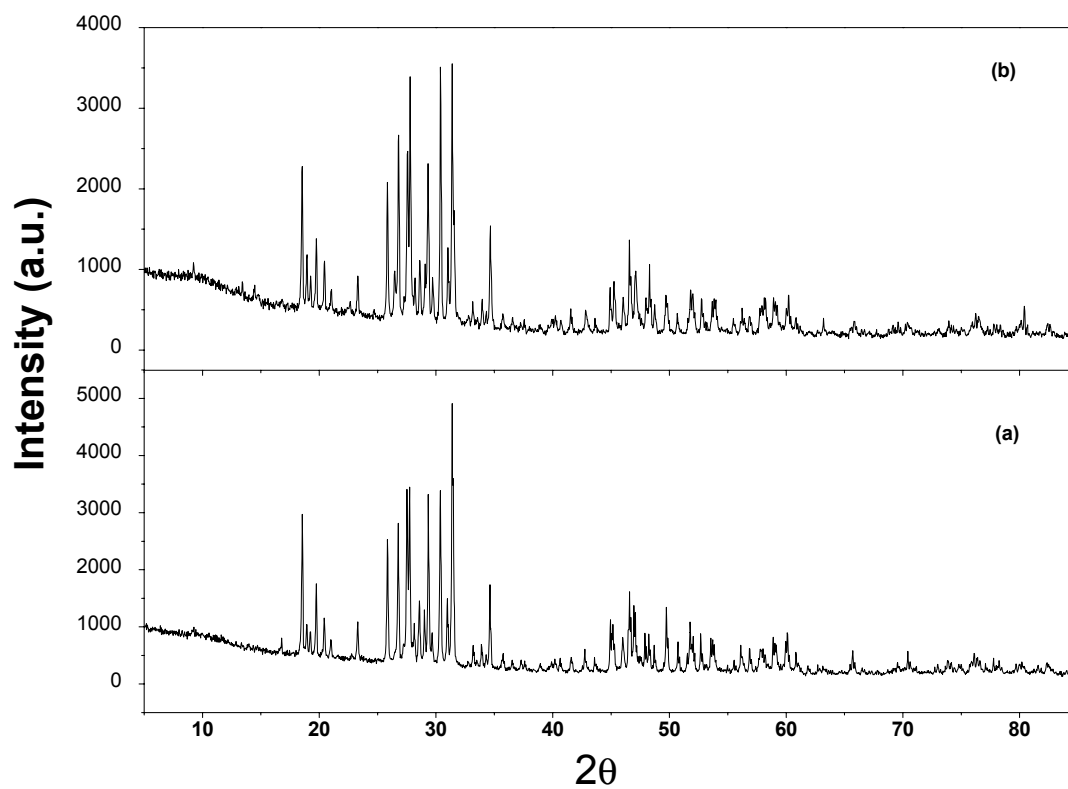


Fig S1. The X-ray powder diffraction patterns of: (a) the as-grown Nd³⁺-doped Li₃Ba₂Y₃(WO₄)₈ crystal from Li₂WO₄; (b) the sample synthesized by solid-state reaction.