Supporting Information

A dual fluorescent/phosphorescent zincophosphite with interesting water adsorption and structural transformation properties

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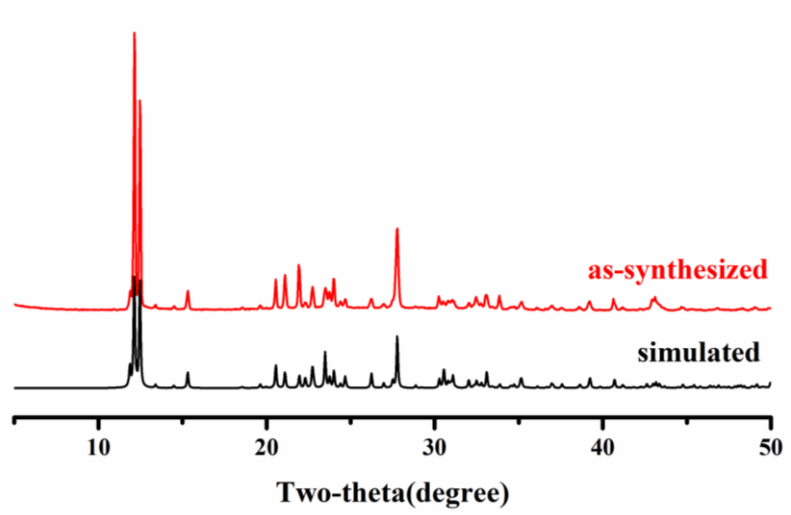

Fig. S1 X-ray powder pattern of **NTOU-6** (top). Powder pattern simulated on the basis of the atomic coordinates derived by single-crystal X-ray diffraction (bottom).

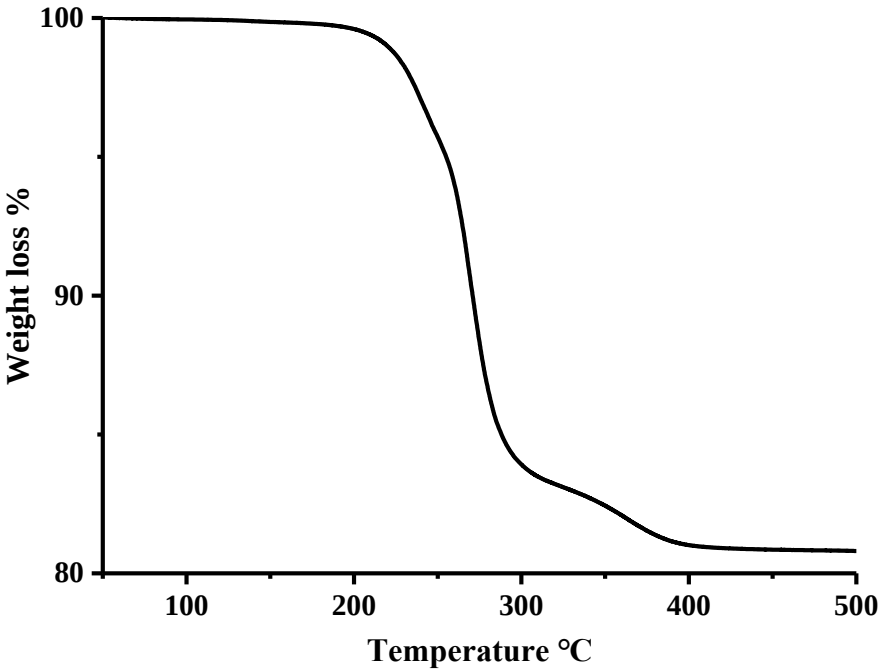

Fig. S2 TGA curve for **NTOU-6** in N_2 at 5 °C min^{-1} from 40 to 550°C.

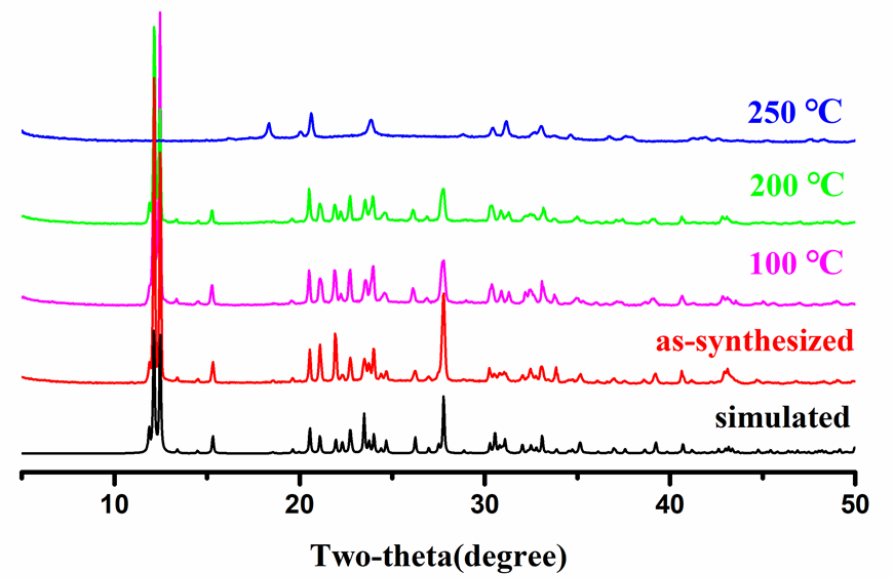

Fig. S3 X-ray powder patterns of **NTOU-6** for thermal-stability testing: simulated, as-synthesized, holding for 1 h at 100℃, 200℃, and 250℃.

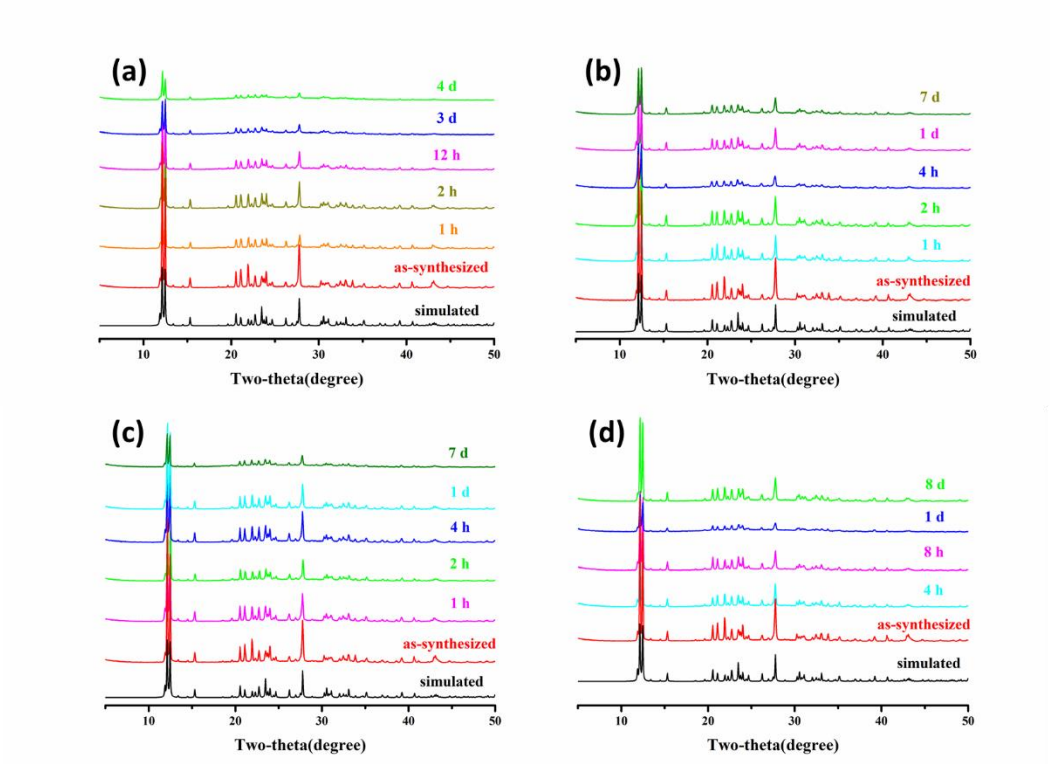

Fig. S4 X-ray powder patterns of **NTOU-6** for chemical-stability studies conducted by suspending the powder samples in organic solvents for several days: (a) hexane, (b) ethanol, (c) methanol, and (d) DMF.

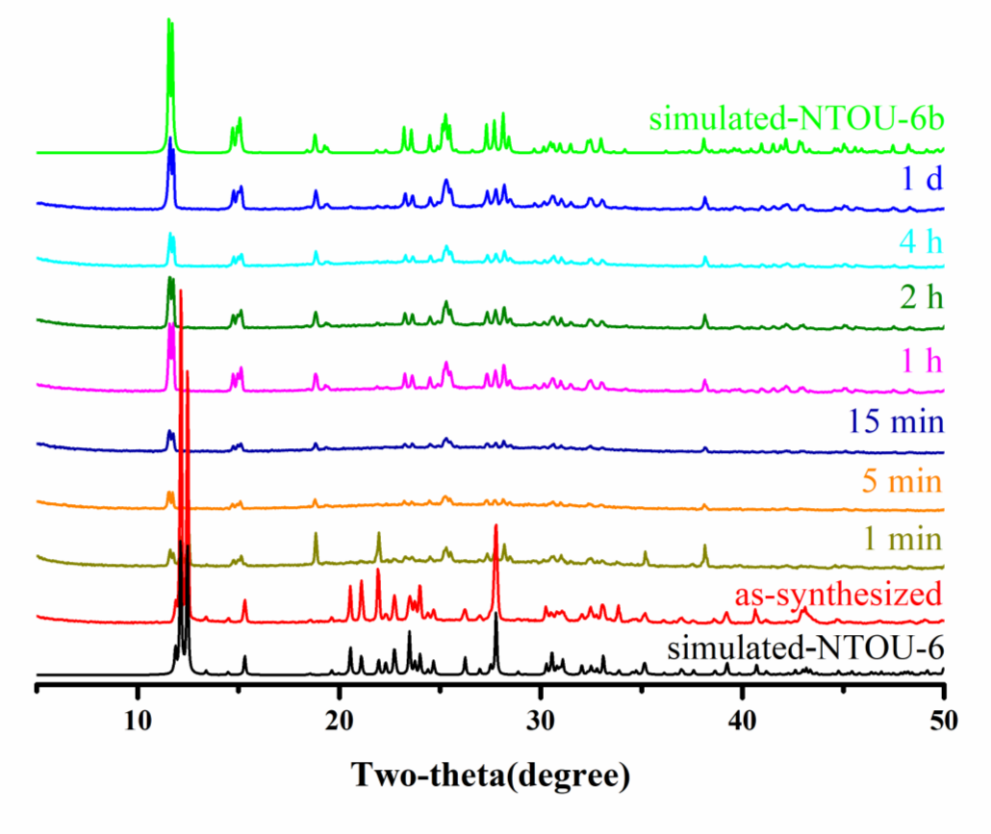

Fig. S5 The X-ray powder patterns of **NTOU-6** for the water-stability testing.

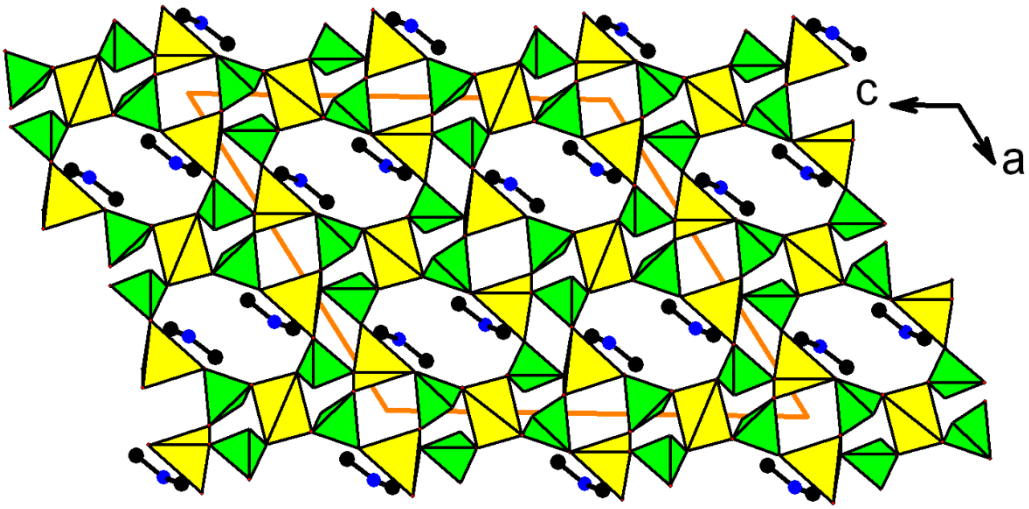

Fig. S6 NTOU-6 with 4-, and 8- member rings alone *b* axis.

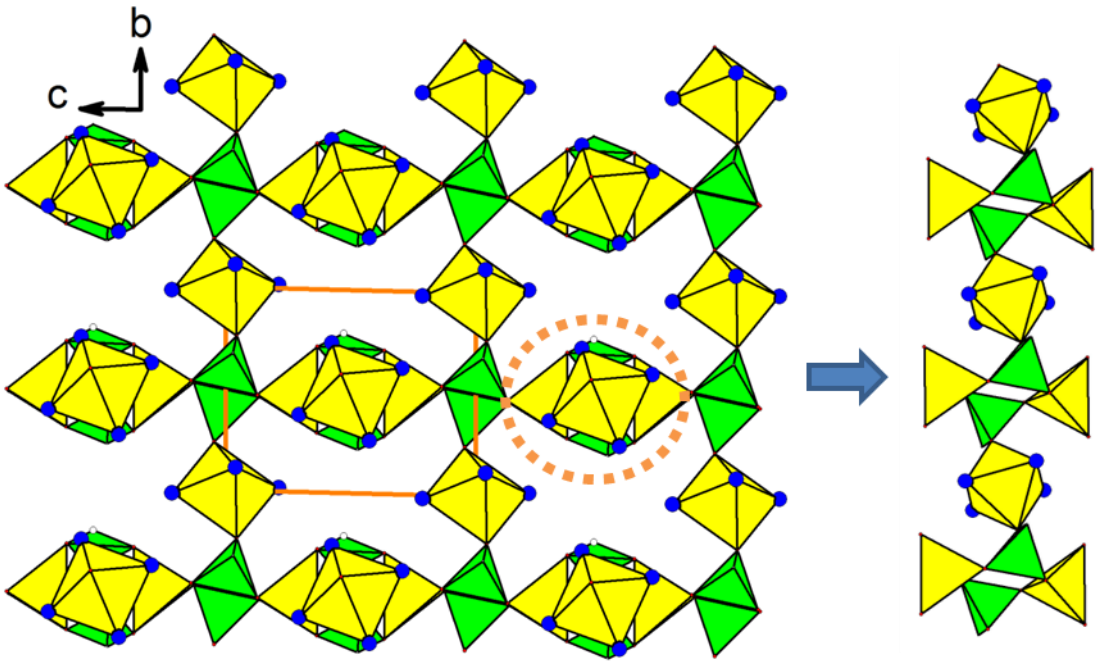

Fig. S7 The 12-membered rings in compound **NTOU-6b** made up of two $[ZnO_2(H_2O)_4]^{2-}$ groups, four ZnO_4 units, and six HPO_3 tetrahedra.

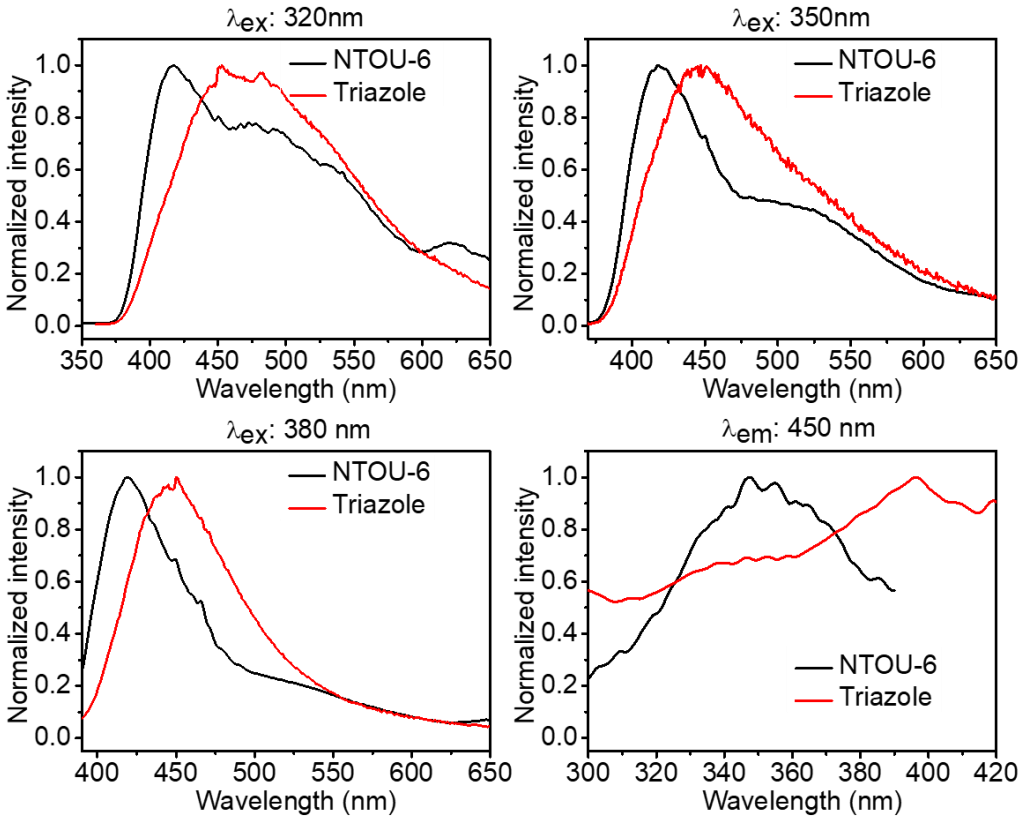

Fig. S8 Comparison of the emission and excitation spectra for the title compound and triazole molecules.

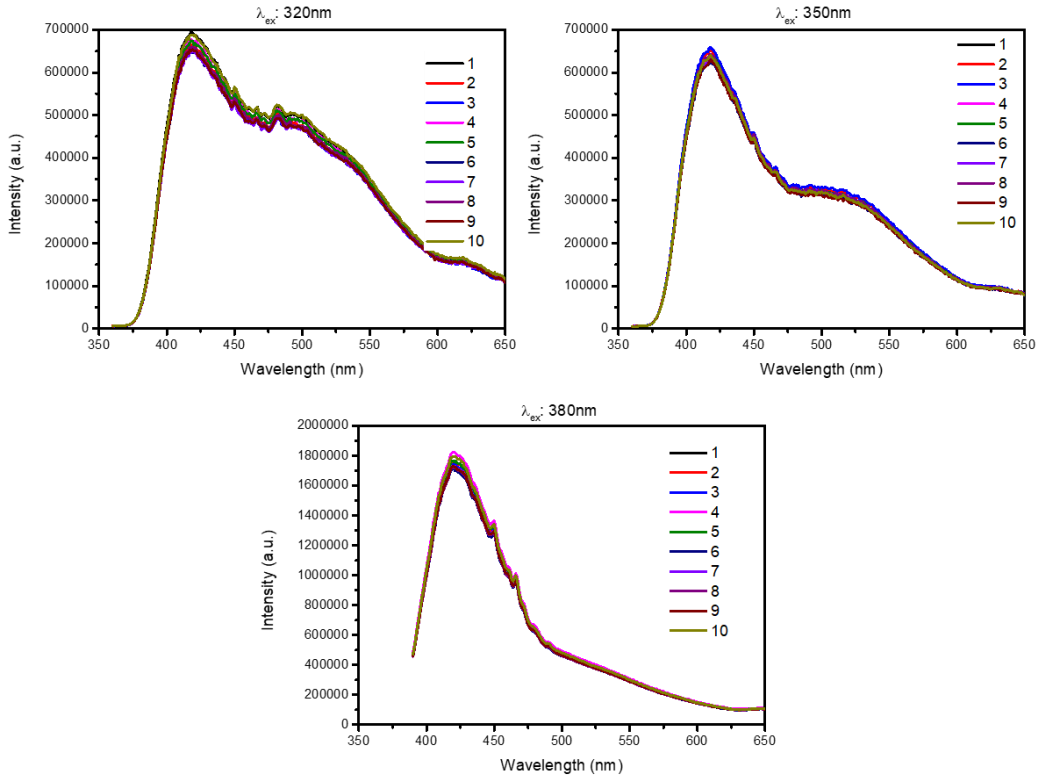

Fig. S9 Emission spectra of repeated excitation showing the photostability of **NTOU-6**.

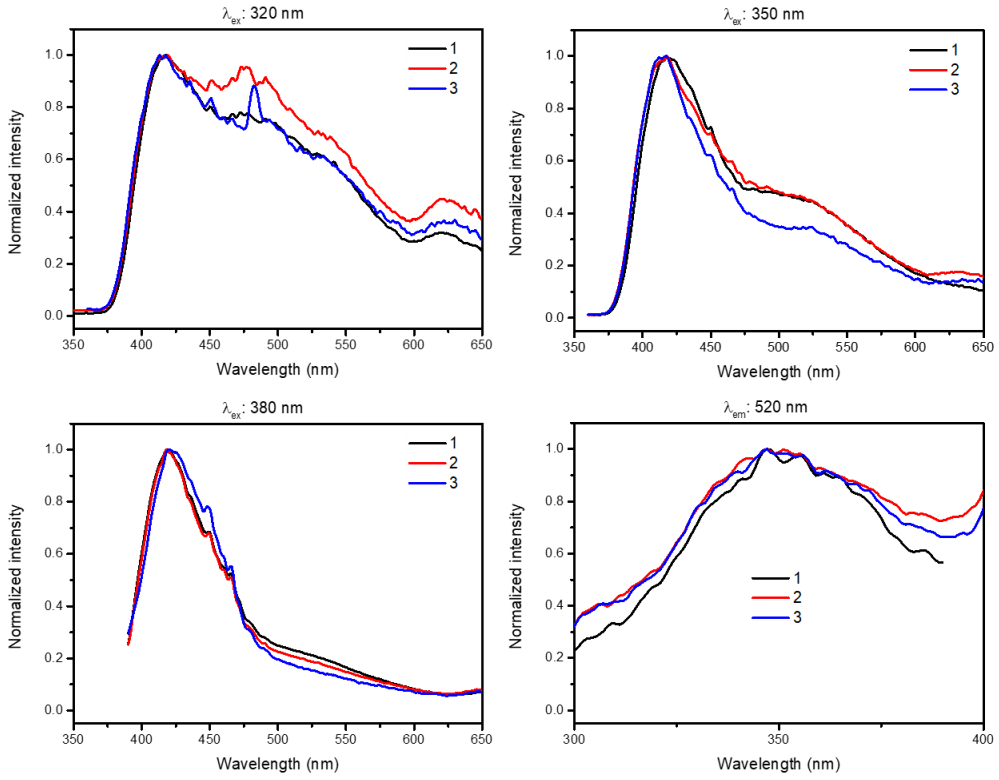

Fig. S10 Reproducibility test for **NTOU-6** at different excitation wavelengths by using different batches.

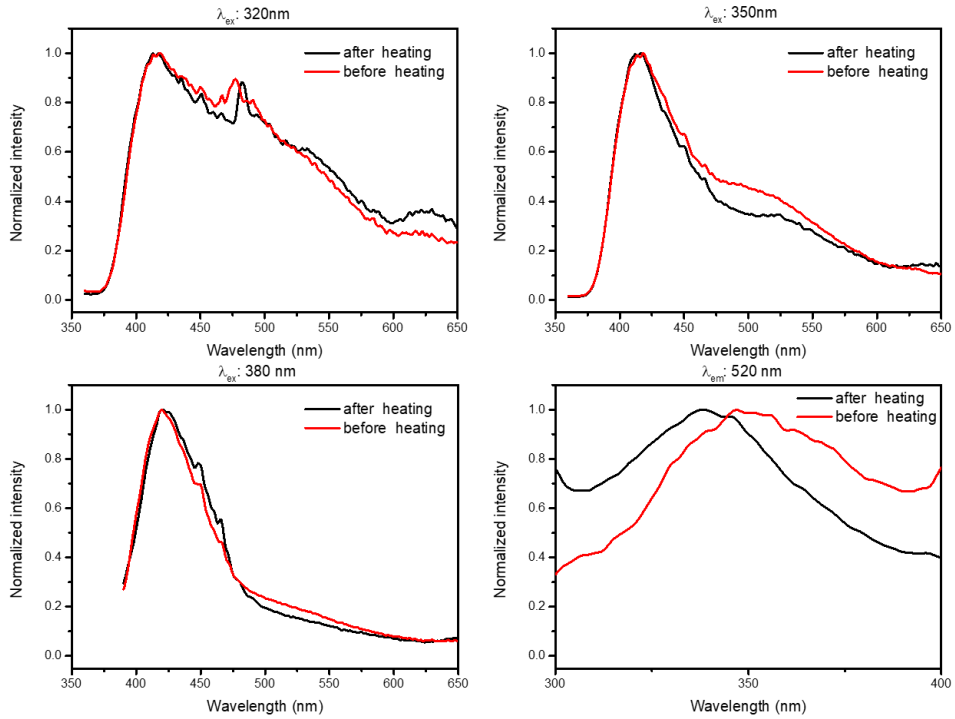

Fig. S11 Thermostability test on **NTOU-6** by comparing the emission spectra before and after heating. Experimental conditions: the compound was heated to 100°C and held for 1 hour, then cooled to room temperature before recording the fluorescence spectra.

Table S1. The lifetime for **NTOU-6** and triazole ligands in the solid state.

Compound	Ex: 350 nm/ Em: 420 nm	Ex: 350 nm/ Em: 520 nm
NTOU-6	1.75 ns	0.9 μs
	χ^2: 1.29	χ^2: 1.20
Triazole	2.79 ns	3.58 ns
	χ^2: 1.25	χ^2: 1.33