Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

A Mixed-Valent Uranium(V, VI) Organic Framework as a Fluorescence Thermometer

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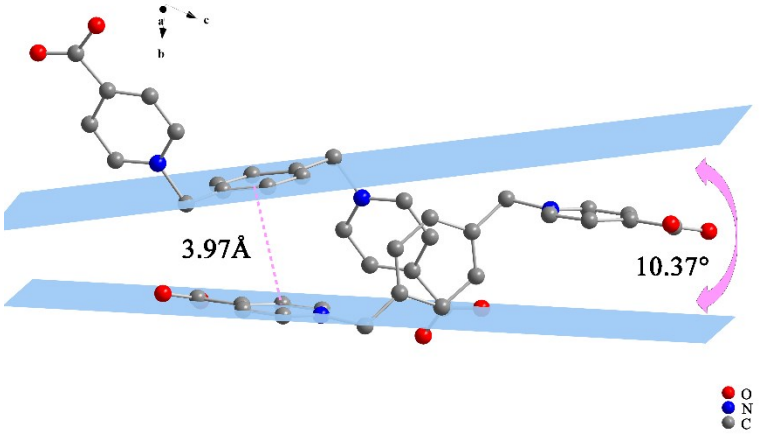

Figure S1 π-π stacking interaction in **HNU-46**. Removal of U and H atoms for easy observation.

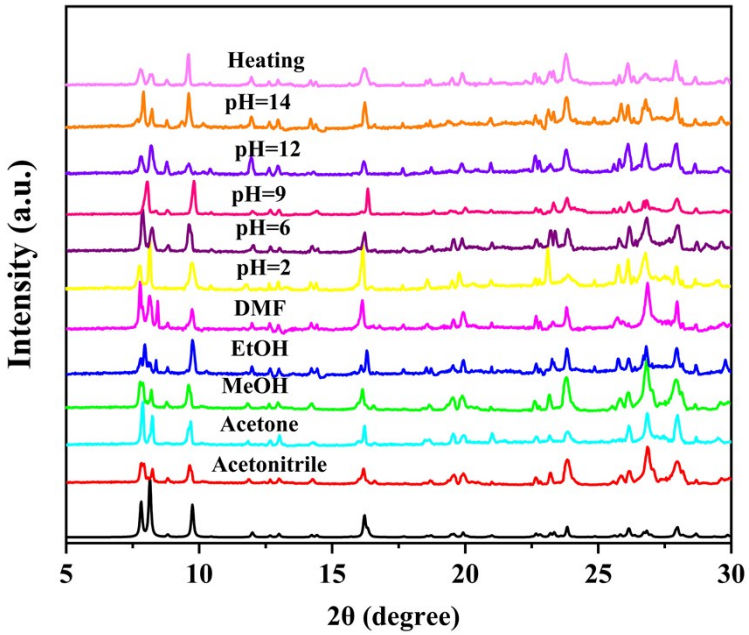

Figure S2 PXRD patterns after immersing **HNU-46** in different solvents for 12h.

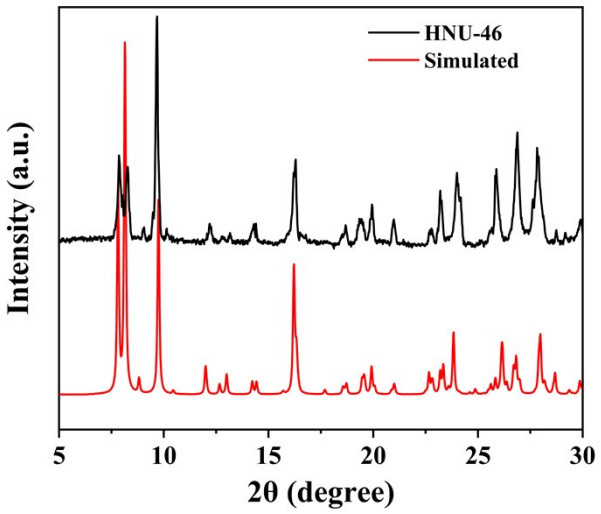

Figure S3 PXRD patterns of synthesized **HNU-46** after one year of storage under air.

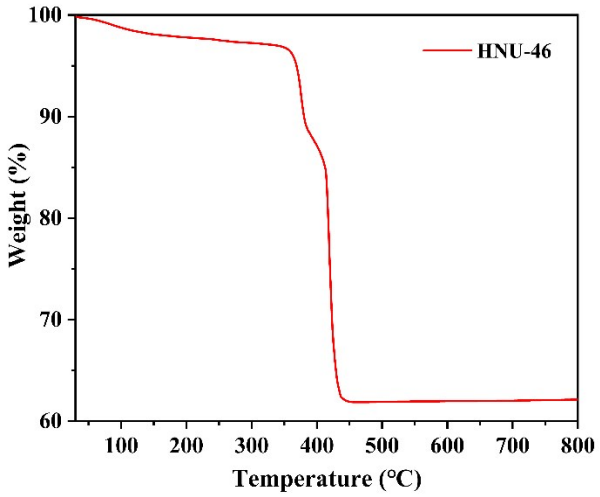

Figure S4 TGA curve of as-synthesized **HNU-46** in air.

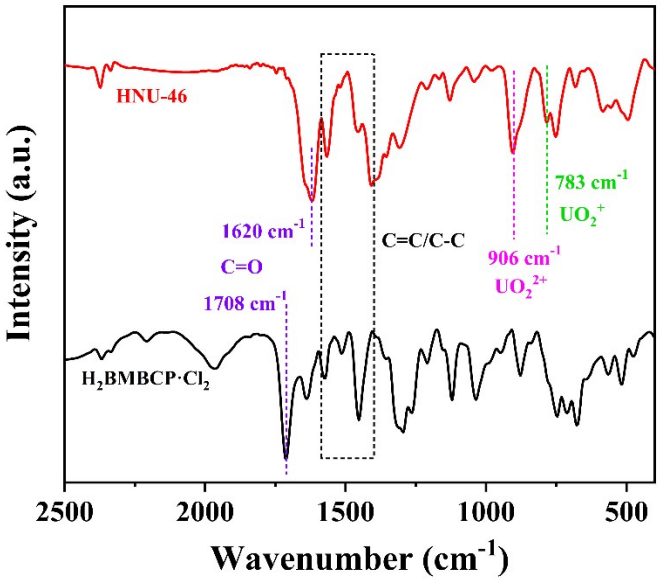

Figure S5 Infrared (IR) spectra of **HNU-46** and $H_2BMBCP{\cdot}Cl_2$ ligand.

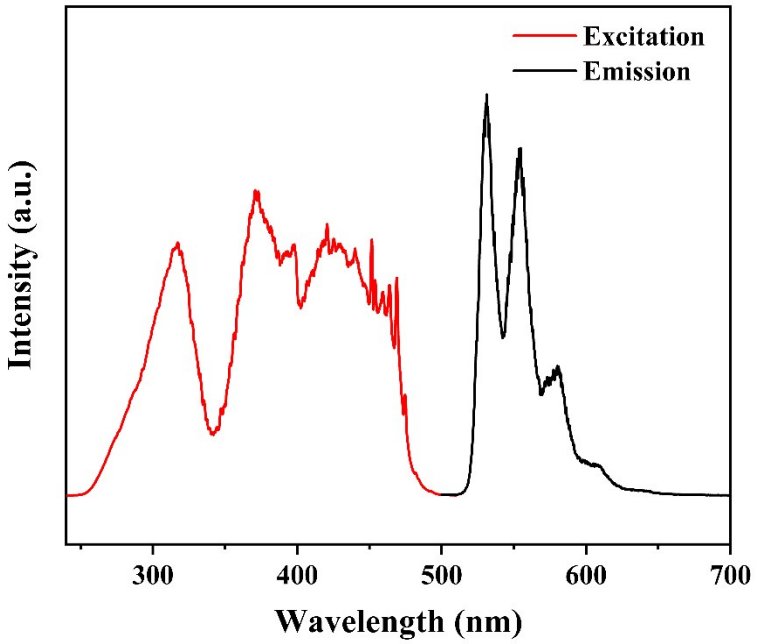

Figure S6 Solid-state excitation and emission spectra of **HNU-46** at 77 K (λ_{em} = 530 nm, λ_{ex} = 370 nm).

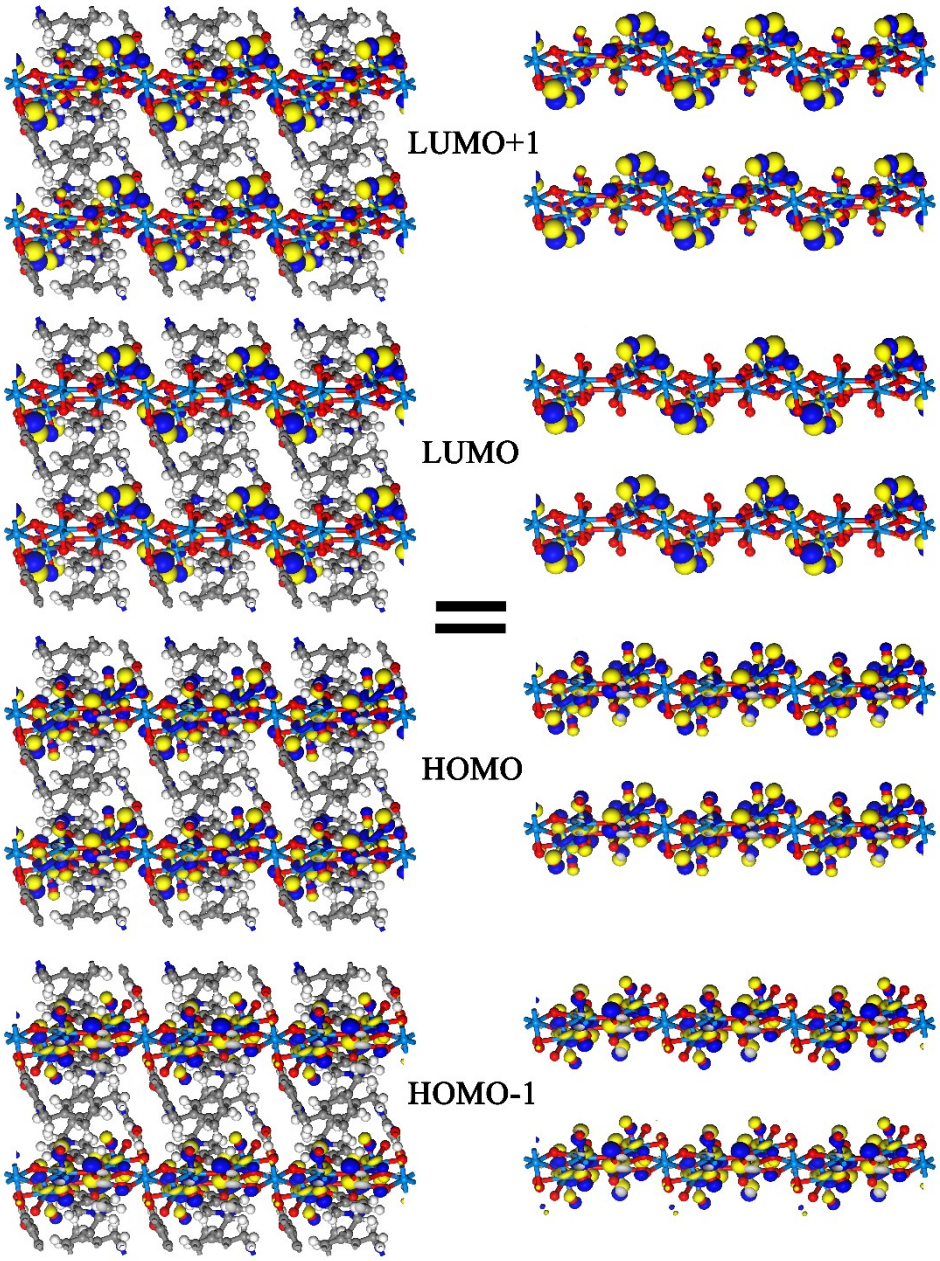

Figure S7 Frontier orbital of **HNU-46** (left) with ligands removed for easier viewing (right).

Table S1 Crystallographic data of **HNU-46**

Complex	**HNU-46**
Formula	$C_{40}H_{32}N_4O_{26}U_5$
*M*r	2174.85
Crystal system	Triclinic
Space group	*P -1*
a(Å)	10.2745(3)
b(Å)	11.2321(4)
c(Å)	11.9901(4)
α(°)	74.880(2)
β(°)	77.193(2)
γ(°)	86.947(2)
V(Å^3)	1302.56(8)
Z	1
D_{calc}(gcm^{-3})	2.773
F(000)	968.0
R_{int}	0.0873
GOF on F^2	1.035
R_1[a][I>2δ(I)]	0.0757
wR_2[b](all data)	0.2195

[a] $R_1 = \sum||F_0|-|F_c||/\sum|F_0|$. [b] $wR_2 = [\sum[w(F_0^2 - F_c^2)^2]/ w(F_0^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_0)^2 + (aP)^2 + bP]$ and $P = (F_0^2 + 2F_c^2)/3$.