

## Supporting Information

# Rare-earth-based donor-acceptor metal-organic frameworks with low thermal quenching and dual emission mechanisms for high-temperature sensing

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# 1. Experimental

## 1.1 Materials and Measurements

All the reagents and solvents employed were commercially purchased and used as received. Emission spectra at room temperature were measured with a Hitachi F4600 luminescence spectrophotometer. Variable-temperature fluorescent spectra, quantum yield and fluorescence lifetime were measured with an Edinburgh FLS980 fluorescence spectrophotometer. Luminescent images were obtained by using an automated Leica DM3000B microscope. Thermogravimetric analyses (TGA) were measured on a METTLER TOLEO TGA/DSC3+ thermo analyzer under nitrogen with a heating rate of  $10\text{ }^{\circ}\text{C min}^{-1}$  between ambient temperature and  $800\text{ }^{\circ}\text{C}$ . Powder X-ray diffraction (PXRD) patterns were collected on a Bruker D8 ADVANCE X-ray diffractometer using Cu-K $\alpha$  radiation ( $\lambda = 0.1542\text{ nm}$ ) over the  $2\theta$  range of  $5\text{--}50^{\circ}$ , in which the X-ray tube was operated at  $40\text{ kV}$  and  $40\text{ mA}$  at room temperature. UV-vis spectra were carried on a SHIMADZU UV-2700 spectrophotometer.

## 1.2 X-ray Crystallography

X-ray diffraction data for the single crystal sample of **DZU-500(M) $\supset$ pyrene** were collected on a vario diffractometer equipped with a graphite monochromated Mo-K $\alpha$  radiation ( $\lambda = 0.71073\text{ \AA}$ ) at room temperature. Absorption corrections were applied by utilizing SADABS routine. The structure dates solved and refined by direct methods and full-matrix least-squares methods on  $F^2$  using the SHEXL-2019. The integrated system of single suite Olex2 was used for the crystallographic programs. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms of which positions and thermal parameters fixed as well as the structure refinement were implemented by geometrically calculations. The crystallographic data are showed in Table S2. The date of relevant bond lengths and angles are listed in Table S3. Notably, the crystal data of **DZU-500(Eu) $\supset$ pyrene-2D** means the crystals of compound 3 were first heated under  $573\text{ K}$  for a while and then the data collection was performed after cooling the crystals to room temperature. As the sample has been heated, this crystal has low quality and is weakly diffracted. Therefore, some crystal problems might be caused by

weak diffraction and disorder.

### **1.3 Synthesis of {[Eu(dppz)(PTA)<sub>1.5</sub>(H<sub>2</sub>O)](dppz)<sub>0.5</sub>}<sub>n</sub> (DZU-500(Eu)⊃pyrene, 3)}**

A mixture of Eu(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (22.7 mg, 0.05 mmol), dppz (8.5 mg, 0.03 mmol) and H<sub>2</sub>PTA (5 mg, 0.03 mmol) and pyrene (3 mg, 0.015 mmol) in a mixture of DMF (0.75 mL), methanol (0.75 mL), water (0.5 mL) was placed in a 4 mL capped vial and heated at 90 °C for 24 h. After cooling to room temperature, orange block crystals of compound **3** were collected by filtration (yield: 58% based on dppz). Elemental analysis (%): calculated for C<sub>38</sub>H<sub>23</sub>N<sub>4</sub>EuO<sub>7</sub>, C 57.08, H 2.89, N 7.01; found: C 56.91, H 2.75, N 7.17.

### **1.4 Synthesis of DZU-500(Eu)⊃guests (1,2,4)**

Compounds **1,2,4** were synthesized similarly to compound **3**, with the introduction of the corresponding guest (0.015 mmol) in the reaction system. For **1** (guest = triphenylene), yellow crystals were obtained. Yield: 62% (based on dppz). For **2** (guest = phenanthrene), light yellow crystals were obtained. Yield: 57% (based on dppz). For **4** (guest = anthracene), orange crystals were obtained. Yield: 60% (based on dppz).

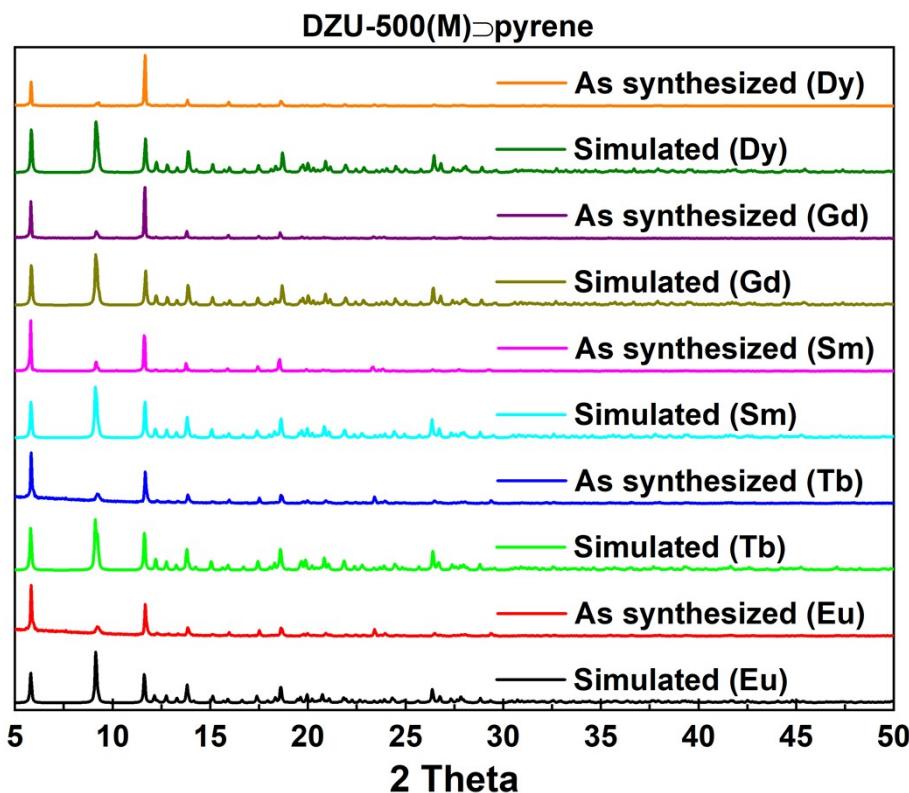
### **1.5 Synthesis of DZU-500(M)⊃pyrene (M= Dy, Gd, Sm, Tb)**

DZU-500(M)⊃pyrene was synthesized similarly to **3**, with the introduction of the corresponding metallic nitrate (0.05 mmol) in the reaction system. All obtained orange block crystals with similar yields.

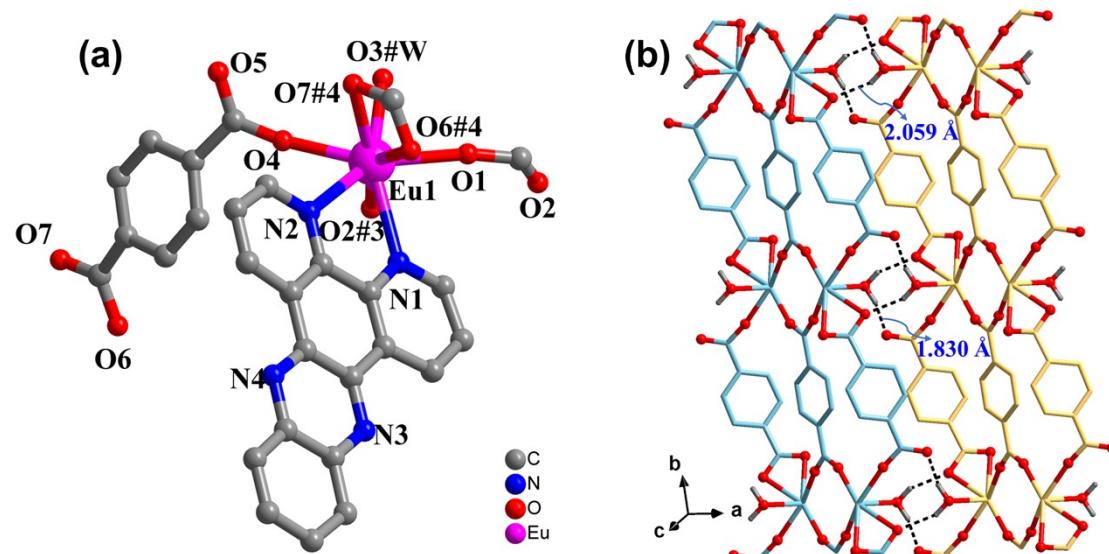
### **1.6 Preparation of the PAN membrane**

A fully ground powder sample of compound **1** (100 mg) was dispersed in DMF (2.5 mL) with the addition of polyacrylonitrile (PAN, 300 mg). The mixture was further magnetically stirred for 48 h, and then added in the injector (5 mL) of the electrospinning machine. During the electrospinning process, the mixture propulsion was kept at a speed of 0.015 mm/min with the voltage around 14 kilovolts. After the mixture was ejected completely, the membrane was taken out and tailored to different forms as desired.

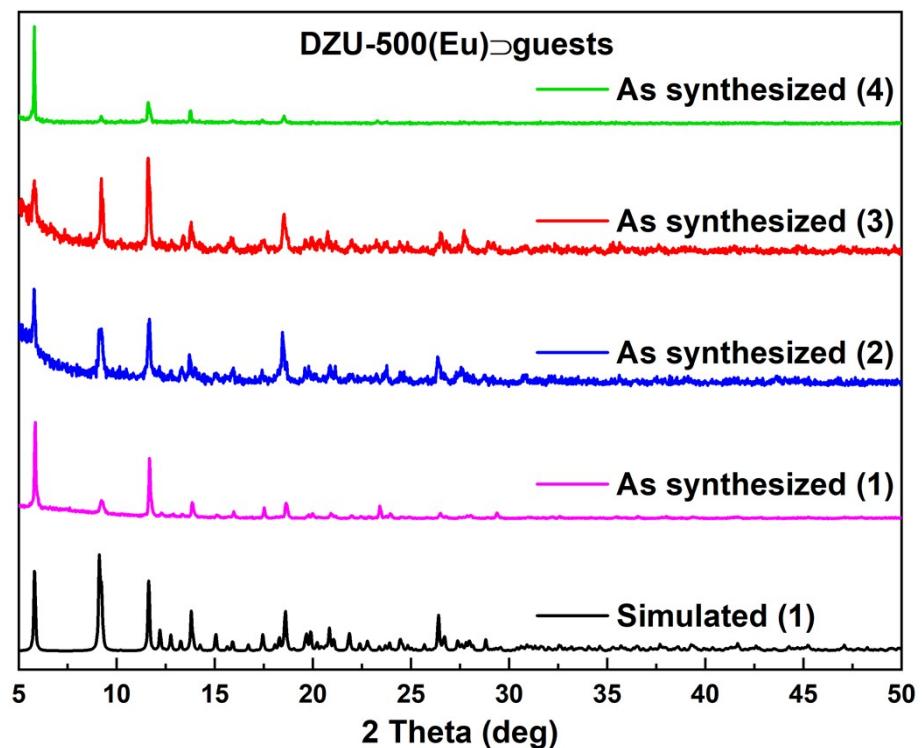
## 2. Addition Figures of the Characterization data.



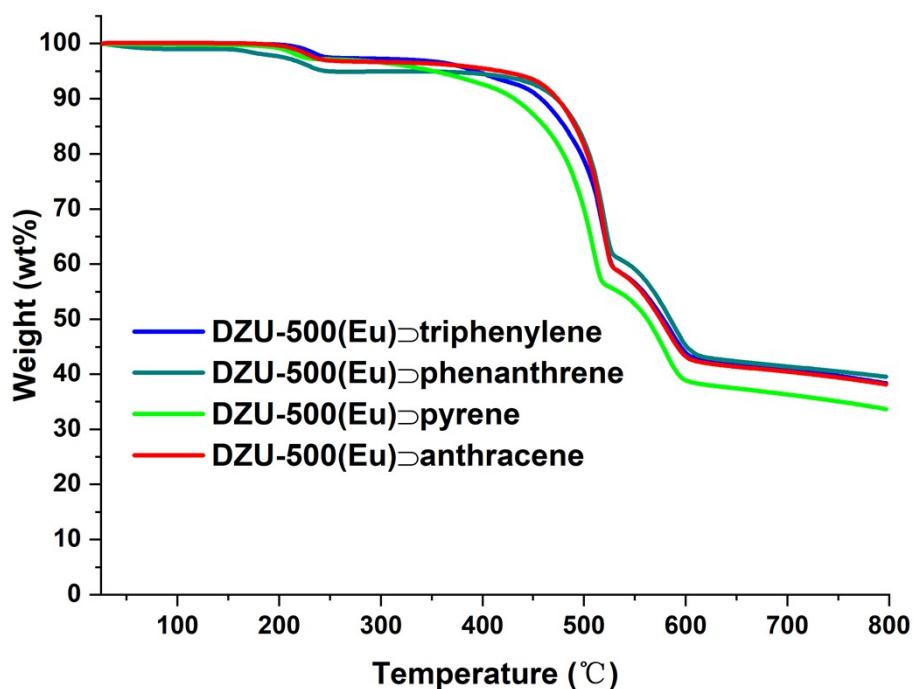
**Fig. S1.** PXRD Patterns of DZU-500-M▫pyrene.



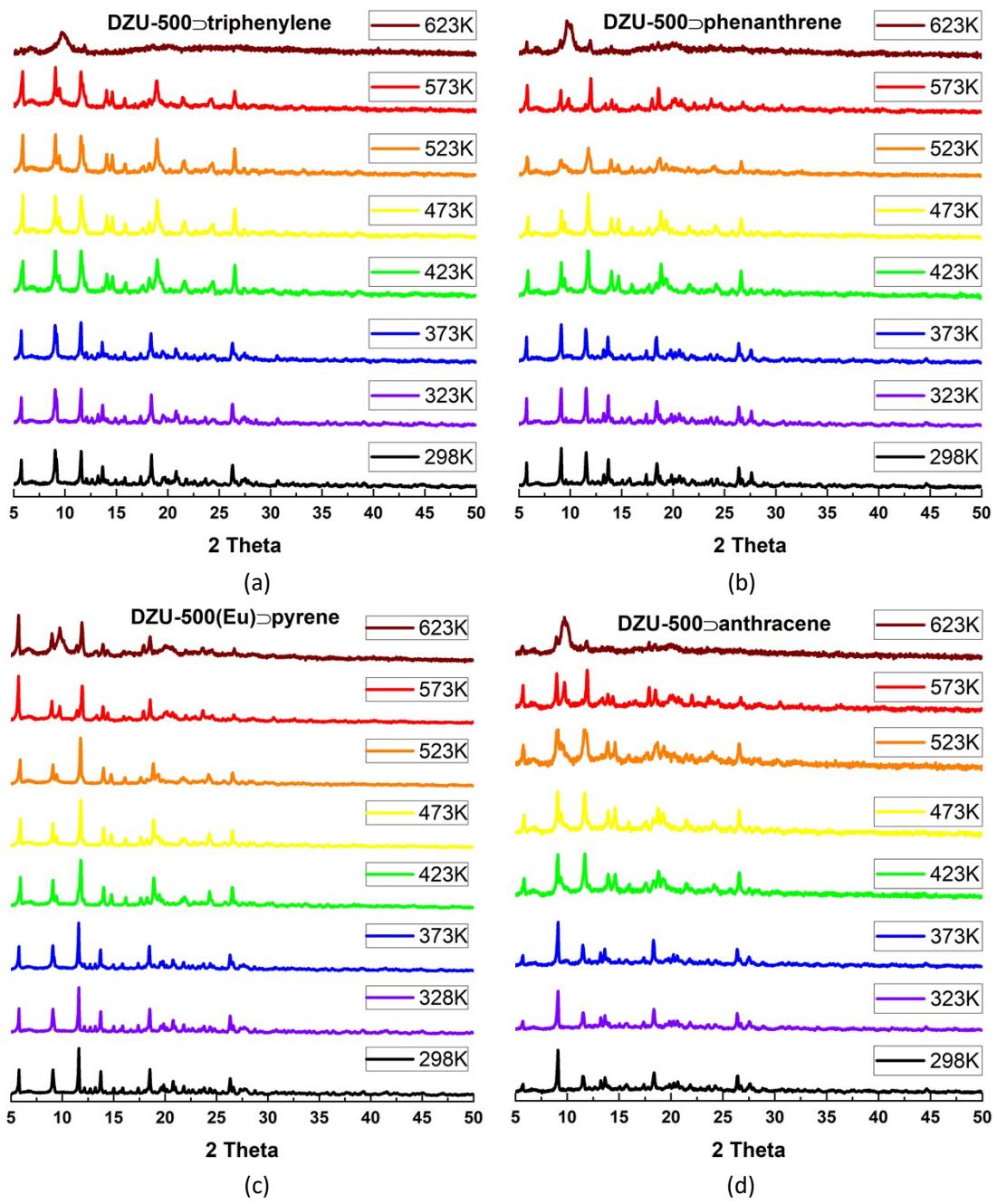
**Fig. S2.** (a) Coordination environments of  $\text{Eu}^{3+}$  ions and (b) the hydrogen bonds in DZU-500(Eu)▫pyrene



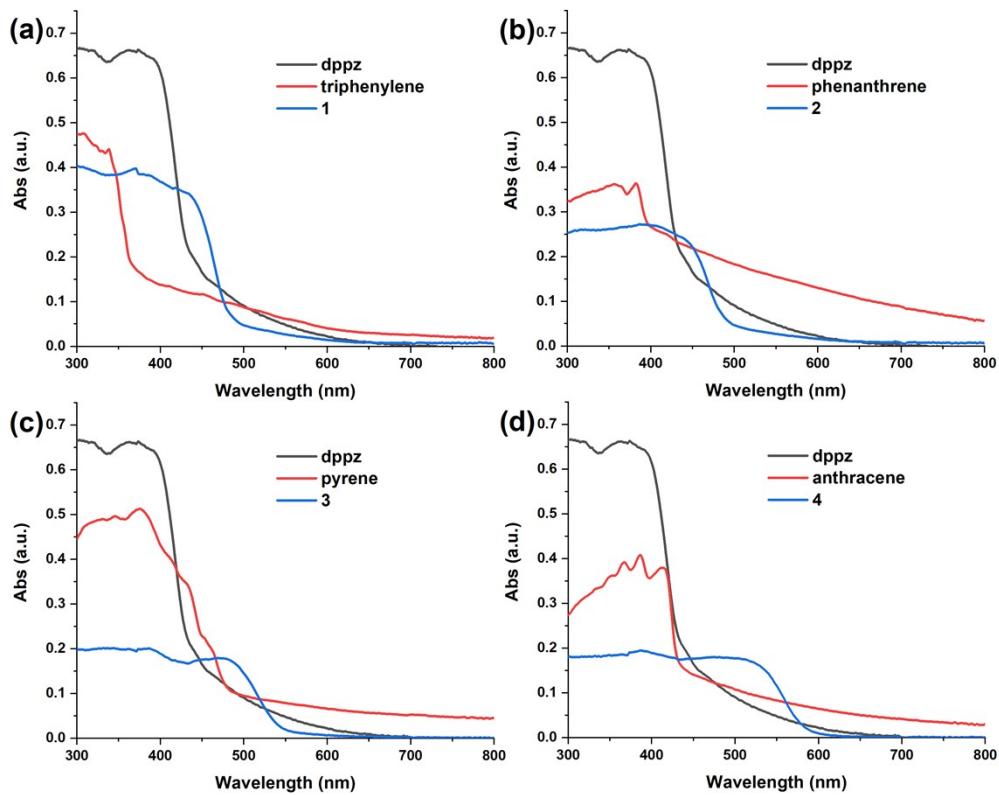
**Fig. S3.** PXRD Patterns of DZU-500(Eu) $\supset$ guests.



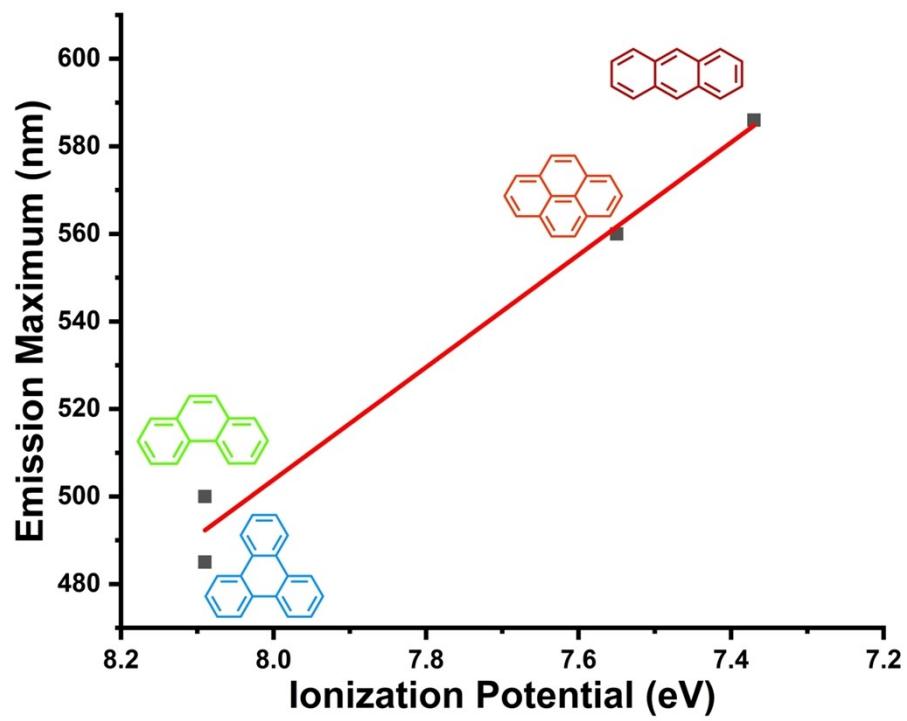
**Fig. S4.** TGA curves of DZU-500(Eu) $\supset$ guests.



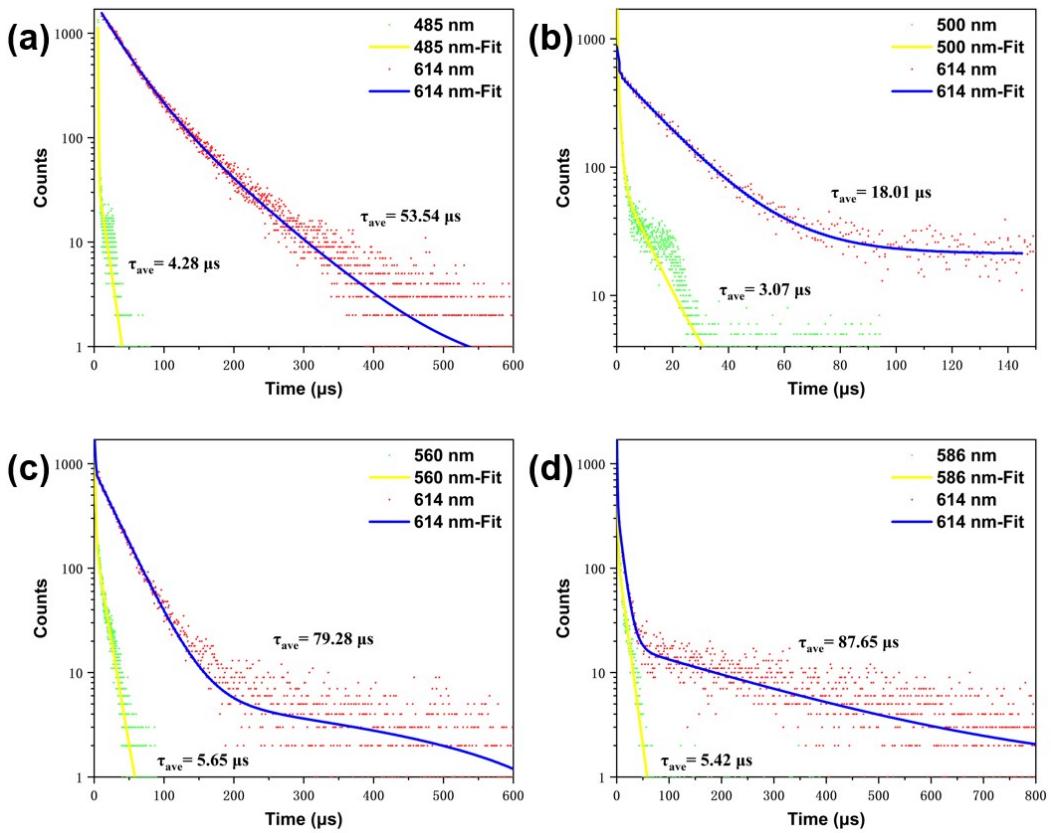
**Fig. S5.** Variable temperature PXRD patterns of DZU-500(Eu)•PAH samples.



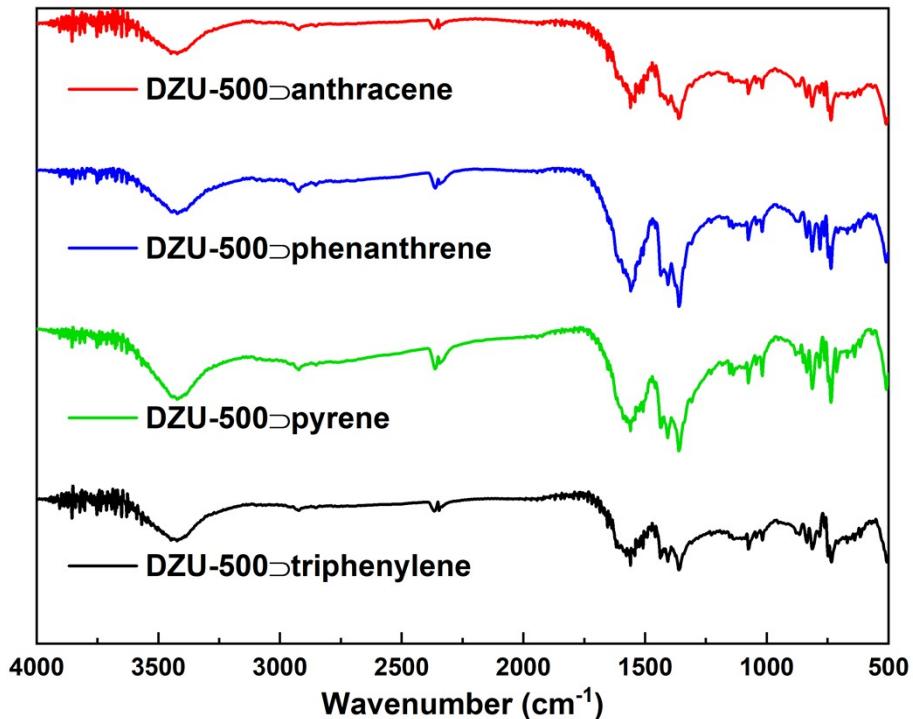
**Fig. S6.** UV-vis spectra of DZU-500(Eu) $\supset$ guests.



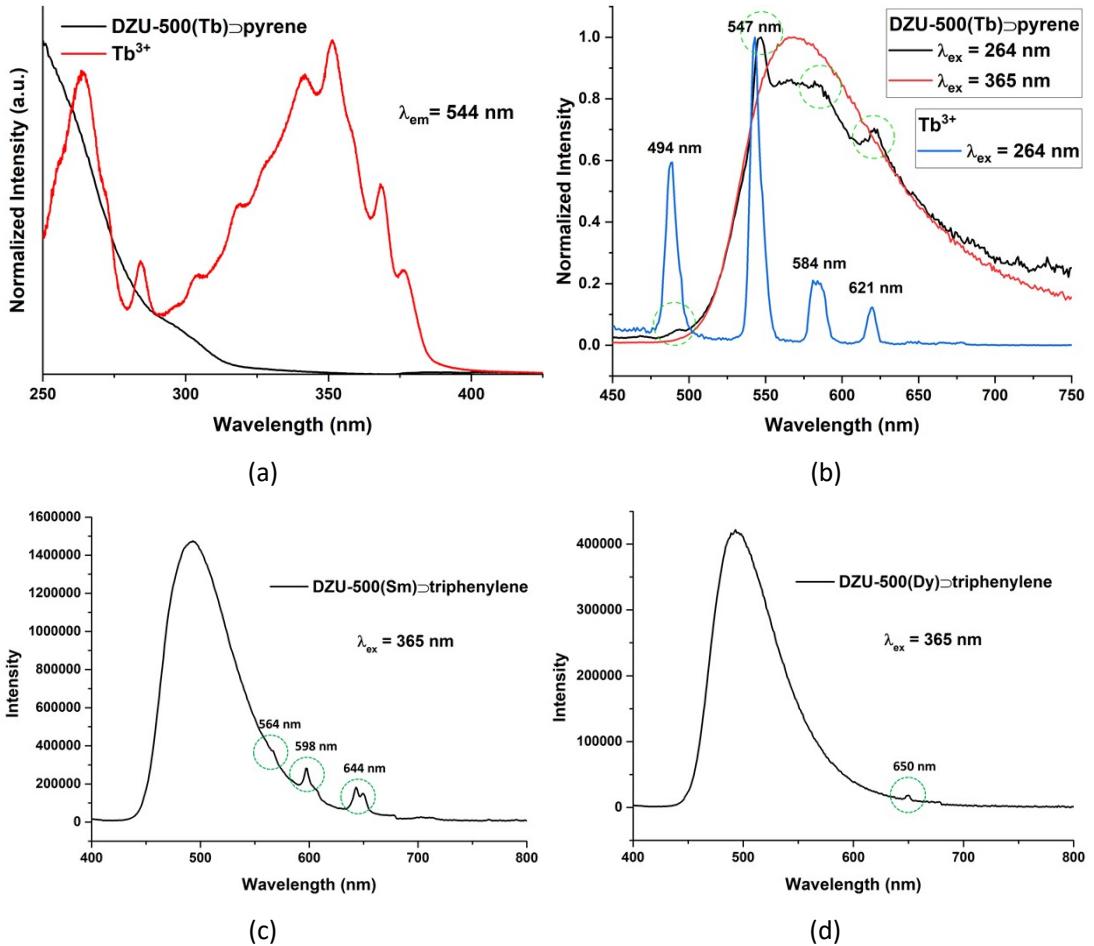
**Fig. S7.** Relationship diagram between the maximum TSCT-based emission wavelength of DZU-500(Eu) $\supset$ guests and the ionization potential of its guest molecules.



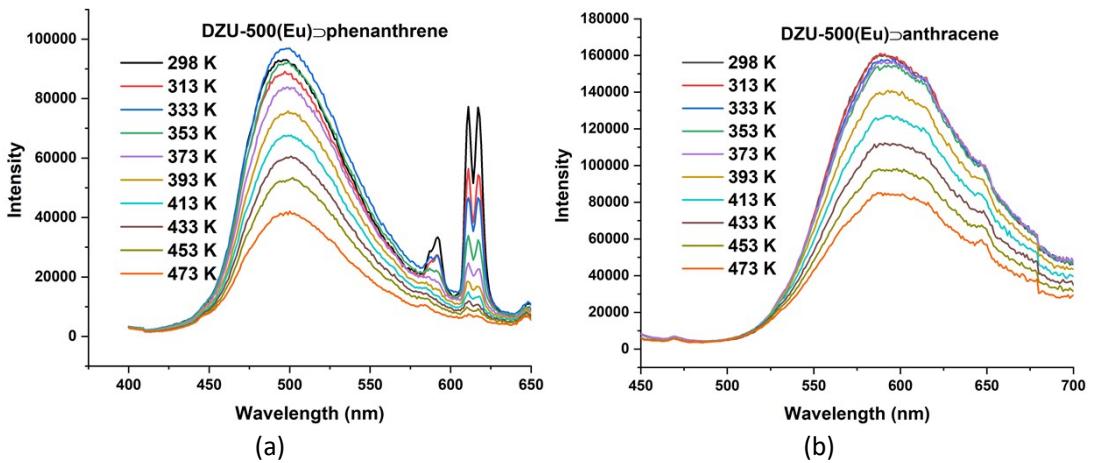
**Fig. S8.** Fluorescence decay curves of (a) DZU-500(Eu) $\supset$ triphenylene, (b) DZU-500(Eu) $\supset$ phenanthrene, (c) DZU-500(Eu) $\supset$ pyrene and (d) DZU-500(Eu) $\supset$ anthracene.



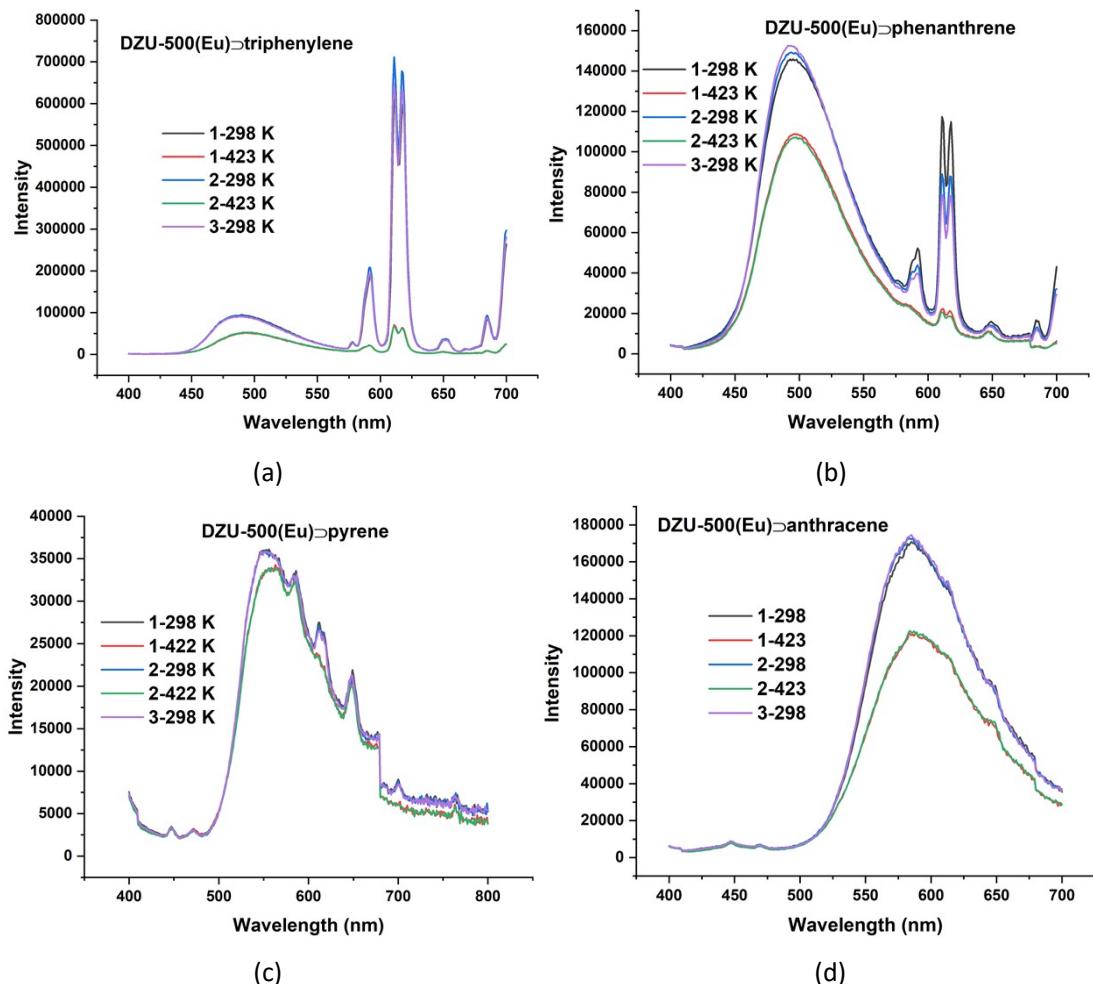
**Fig. S9.** Infrared spectroscopy of the DZU-500(Eu) $\supset$ PAH samples.



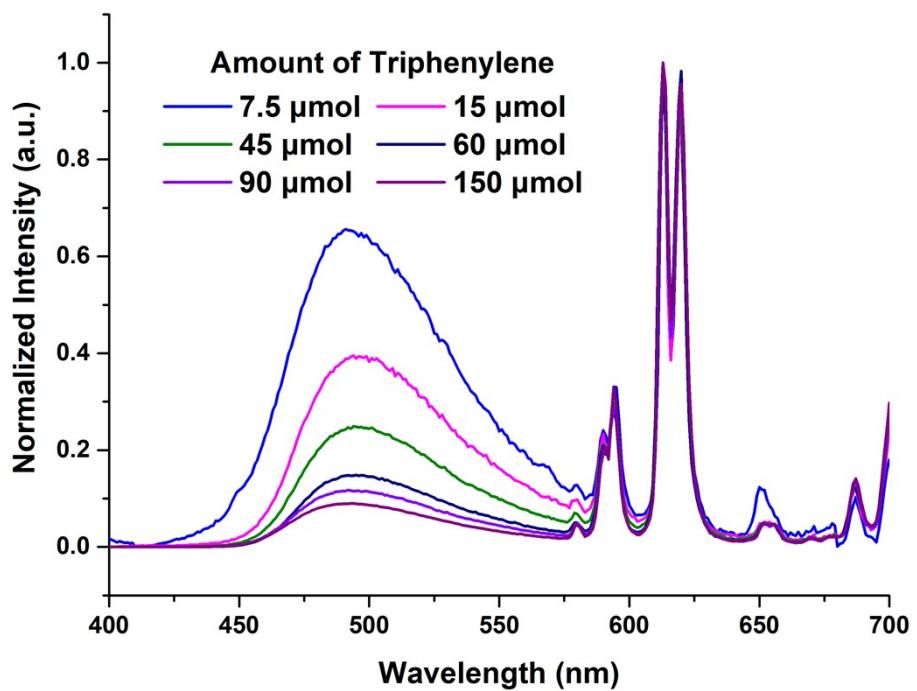
**Fig. S10.** (a) Excitation spectra, and (b) emission spectra of DZU-500(Eu) $\supset$ pyrene, and Tb $^{3+}$  ions; Emission spectra of (c) DZU-500(Sm) $\supset$ triphenylene and (d) DZU-500(Dy) $\supset$ triphenylene.



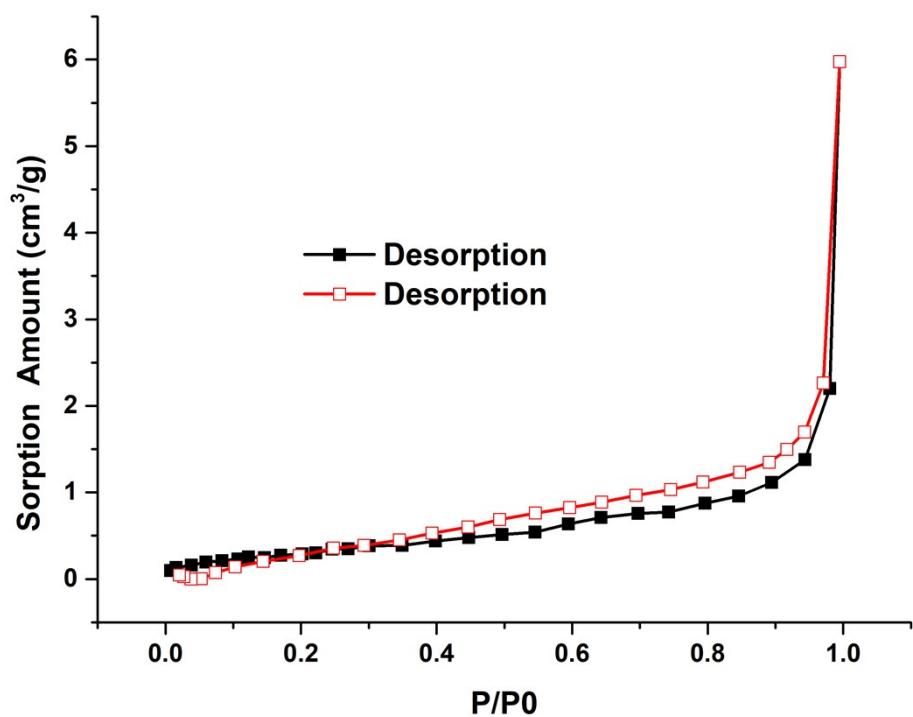
**Fig. S11.** Variable-temperature solid-state emission spectra of (a) DZU-500(Eu) $\supset$ phenanthrene, and (b) DZU-500(Eu) $\supset$ anthracene.



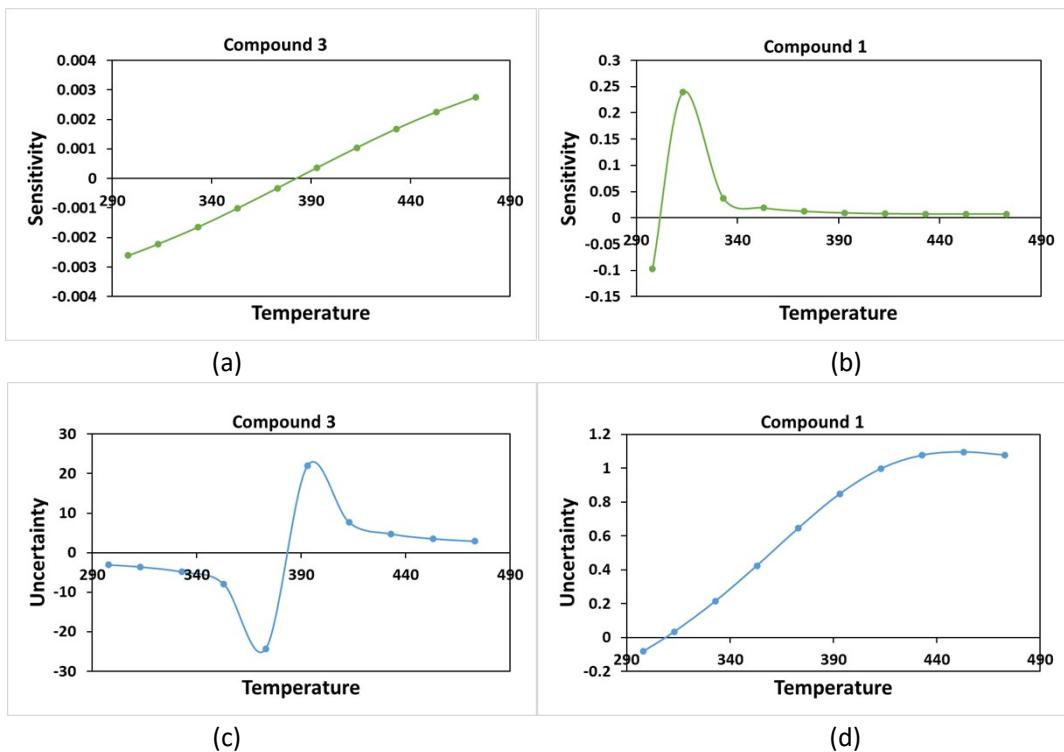
**Fig. S12.** Temperature cycling of the fluorescence of these DZU-500(Eu) $\supset$ PAH samples.



**Fig. S13.** Solid-state emission spectra of samples of DZU-500(Eu)·triphenylene with different loading amount of triphenylene. (dppz: 150  $\mu\text{mol}$ ; TPA: 150  $\mu\text{mol}$ )



**Fig. S14.** N<sub>2</sub> sorption isotherms of compound 3 at 77 K.



**Fig. S15.** (a, b) Relative thermal sensitivity of compound 3 and 1 obtained from Fig. 5d and e. (a)  $S_r(3) = (4E-5T - 0.0153)/(2E-5T^2 - 0.0153T + 4.0793)$ ; (b)  $S_r(1) = (-9E-6T^2 + 0.0072T - 1.5421)/(-3E-6T^3 + 0.0036T^2 - 1.5421T + 221.27)$ . (c, d) Temperature uncertainty ( $\delta_T$ ) of compound 3 and 1. (c)  $\delta_T(3) = 0.8\%/(4E-5T - 0.0153)*(2E-5T^2 - 0.0153T + 4.0793)$ ; (d)  $\delta_T(1) = 0.8\%/(-9E-6T^2 + 0.0072T - 1.5421)*(-3E-6T^3 + 0.0036T^2 - 1.5421T + 221.27)$ .

### 3. Addition Tables of the Characterization data.

Table S1. Summary of Solid-State Luminescent Data for DZU-500 $\supset$ guests.

Coordination polymer	$\lambda_{\text{ex}}$ (nm)	$\lambda_{\text{em-max}}$ (nm)	CIE	$\Phi_{\text{fl}}$ (%)	$\text{av } \tau_{\text{TSCT}}$ ( $\mu\text{s}$ )	$\text{av } \tau_{614 \text{ nm}}$ ( $\mu\text{s}$ )
1	380	485	(0.40, 0.41)	2.52	4.28	53.54
2	380	500	(0.26, 0.44)	0.97	3.07	18.01
3	380	560	(0.45, 0.45)	0.91	5.65	79.28
4	380	586	(0.45, 0.35)	0.72	5.42	87.65

Table S2. Crystal data and structure refinements of DZU-500(M) $\supset$ pyrene.

Compound	<b>3</b>	DZU-500(Dy) $\supset$ pyrene	DZU-500(Gd) $\supset$ pyrene
Empirical formula	$\text{C}_{38}\text{H}_{23}\text{EuN}_4\text{O}_7$	$\text{C}_{38}\text{H}_{23}\text{DyN}_4\text{O}_7$	$\text{C}_{38}\text{H}_{23}\text{GdN}_4\text{O}_7$
Formula weight	799.56	810.10	804.85
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
<i>a</i> ( $\text{\AA}$ )	9.6484(10)	9.6303(4)	9.6322(5)
<i>b</i> ( $\text{\AA}$ )	10.2129(11)	10.1848(4)	10.2018(5)
<i>c</i> ( $\text{\AA}$ )	16.1553(18)	16.0924(7)	16.1078(9)
$\alpha$ ( $^\circ$ )	108.345(5)	71.652(2)	71.546(2)
$\beta$ ( $^\circ$ )	96.400(5)	80.612(2)	80.518(2)
$\gamma$ ( $^\circ$ )	95.058(6)	84.991(2)	84.977(2)
<i>V</i> ( $\text{\AA}^3$ )	1488.7(3)	1476.99(11)	1479.88(14)
<i>Z</i>	2	2	2
$D_c$ ( $\text{g cm}^{-3}$ )	1.784	1.822	1.806
<i>F</i> (000)	796.0	802.0	798.0
$2\vartheta$ range for data collection ( $^\circ$ )	5.828 to 137.014	2.694 to 54.744	4.212 to 58.636
Goodness-of-fit on $F^2$	1.154	1.162	1.041
Final R indexes [ $ I >=2\sigma( I )$ ]	$R_1 = 0.0370$ , $wR_2 = 0.0845$	$R_1 = 0.0328$ , $wR_2 = 0.0845$	$R_1 = 0.0396$ , $wR_2 = 0.0888$
Final R indexes [all data]	$R_1 = 0.0490$ , $wR_2 = 0.1018$	$R_1 = 0.0360$ , $wR_2 = 0.0858$	$R_1 = 0.0493$ , $wR_2 = 0.0944$
Largest difference in peak and hole ( $e \text{\AA}^{-3}$ )	1.15/-1.76	1.00/-1.18	0.79/-0.99

Compound	DZU-500(Sm)⊂Pyrene	DZU-500(Tb)⊂Pyrene	DZU-500(Eu)⊂Pyrene(373K)
Empirical formula	C <sub>38</sub> H <sub>23</sub> SmN <sub>4</sub> O <sub>7</sub>	C <sub>38</sub> H <sub>23</sub> TbN <sub>4</sub> O <sub>7</sub>	C <sub>38</sub> H <sub>23</sub> EuN <sub>4</sub> O <sub>7</sub>
Formula weight	797.95	806.52	799.56
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
<i>a</i> (Å)	9.6604(6)	9.6431(15)	9.683(3)
<i>b</i> (Å)	10.2260(6)	10.1993(15)	10.224(3)
<i>c</i> (Å)	16.1551(10)	16.139(3)	16.295(4)
$\alpha$ (°)	108.412(2)	108.487(6)	71.877(9)
$\beta$ (°)	96.312(2)	96.165(7)	80.466(9)
$\gamma$ (°)	95.045(2)	94.917(6)	84.587(10)
<i>V</i> (Å <sup>3</sup> )	1492.26(16)	1484.6(4)	1510.5(7)
<i>Z</i>	2	2	2
D <sub>c</sub> (g cm <sup>-3</sup> )	1.776	1.804	1.758
<i>F</i> (000)	794.0	800.0	796.0
2θ range for data collection (°)	4.278 to 54.966	5.834 to 137.144	4.196 to 55.586
Goodness-of-fit on F <sup>2</sup>	1.032	1.107	1.076
Final R indexes [I>=2σ (I)]	R <sub>1</sub> = 0.0441, wR <sub>2</sub> = 0.1073	R <sub>1</sub> = 0.0358, wR <sub>2</sub> = 0.1002	R <sub>1</sub> = 0.0548, wR <sub>2</sub> = 0.1318
Final R indexes [all data]	R <sub>1</sub> = 0.0540, wR <sub>2</sub> = 0.1144	R <sub>1</sub> = 0.0399, wR <sub>2</sub> = 0.1086	R <sub>1</sub> = 0.0822, wR <sub>2</sub> = 0.1482
Largest difference in peak and hole (e Å <sup>-3</sup> )	0.72/-0.88	0.92/-1.41	1.32/-1.28

Compound	DZU-500(Eu)⊃Pyrene(423K)	DZU-500(Eu)⊃Pyrene-2D
Empirical formula	C <sub>38</sub> H <sub>23</sub> EuN <sub>4</sub> O <sub>7</sub>	C <sub>38</sub> H <sub>21</sub> EuN <sub>4</sub> O <sub>6</sub>
Formula weight	799.56	781.55
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
<i>a</i> (Å)	9.7057(4)	9.612(3)
<i>b</i> (Å)	10.2452(5)	10.220(3)
<i>c</i> (Å)	16.2891(7)	15.860(5)
$\alpha$ (°)	72.1450(10)	72.008(8)
$\beta$ (°)	80.5120(10)	78.487(8)
$\gamma$ (°)	84.9320(10)	79.532(7)
<i>V</i> (Å <sup>3</sup> )	1519.40(12)	1439.9(8)
<i>Z</i>	2	2
D <sub>c</sub> (g cm <sup>-3</sup> )	1.748	1.803
<i>F</i> (000)	796.0	776.0
2θ range for data collection (°)	4.234 to 55.028	4.226 to 45.994
Goodness-of-fit on F <sup>2</sup>	1.059	1.101
Final R indexes [I>=2σ (I)]	R <sub>1</sub> = 0.0343, wR <sub>2</sub> = 0.0843	R <sub>1</sub> = 0.0984, wR <sub>2</sub> = 0.2686
Final R indexes [all data]	R <sub>1</sub> = 0.0439, wR <sub>2</sub> = 0.0904	R <sub>1</sub> = 0.1347, wR <sub>2</sub> = 0.2913
Largest difference in peak and hole (e Å <sup>-3</sup> )	0.96/-0.78	4.20/-1.78

**Table S3.** Selected Bond Lengths [Å] and Bond Angles [deg] for the DZU-500(M)⊃pyrene.

DZU-500(Dy)⊃Pyrene			
Dy1-N1	2.530(3)	O(1)-Dy(1)-O(5)#1	150.09(10)
Dy1-N2	2.576(3)	O(1)-Dy(1)-O(6)#1	155.82(11)
Dy1-O1	2.320(3)	O(1)-Dy(1)-O(7)	84.88(11)
Dy1-O2#1	2.311(3)	O(1)-Dy(1)-N(1)	76.00(11)
Dy1-O3	2.253(3)	O(1)-Dy(1)-N(2)	110.78(11)
Dy1-O5#2	2.468(3)	O(2)#2-Dy(1)-O(1)	86.40(11)
Dy1-O6#2	2.440(3)	O(2)#2-Dy(1)-O(5)#1	75.18(11)
Dy1-O7	2.356(3)	O(2)#2-Dy(1)-O(6)#1	100.25(10)
O(2)#2-Dy(1)-O(7)	75.18(10)	O(2)#2-Dy(1)-N(1)	82.00(11)
O(2)#2-Dy(1)-N(2)	134.95(11)	O(3)-Dy(1)-O(1)	82.79(11)
O(3)-Dy(1)-O(2)#2	152.20(12)	O(3)-Dy(1)-O(5)#1	123.66(11)
O(3)-Dy(1)-O(6)#1	80.68(10)	O(3)-Dy(1)-O(7)	78.39(11)
O(3)-Dy(1)-N(1)	119.62(11)	O(3)-Dy(1)-N(2)	72.82(11)
O(5)#1-Dy(1)-N(1)	78.22(11)	O(5)#1-Dy(1)-N(2)	69.97(11)
O(6)#1-Dy(1)-O(5)#1	53.09(10)	O(6)#1-Dy(1)-N(1)	127.76(11)

O(6)#1-Dy(1)-N(2)	80.92(11)	O(7)-Dy(1)-O(5)#1	112.06(10)
O(7)-Dy(1)-O(6)#1	74.61(10)	O(7)-Dy(1)-N(1)	151.03(11)
O(7)-Dy(1)-N(2)	144.72(10)	N(1)-Dy(1)-N(2)	63.85(11)

Symmetry codes #1: 1-X,-Y,2-Z; #2: X,-1+Y,Z; #3: X,1+Y,Z; #4: 1-X,1-Y,2-Z; #5: 1-X,2-Y,1-Z;

#### DZU-500(Eu)⊂Pyrene(373K)

Eu1-O1	2.278(5)	O1-Eu1O3#1	122.1(2)
Eu1-O3#1	2.485(5)	O1-Eu1-O4#1	79.70(19)
Eu1-O4#1	2.486(5)	O1-Eu1-O5	152.4(2)
Eu1-O5	2.345(5)	O1-Eu1-O6#2	83.8(2)
Eu1-O6#2	2.352(5)	O1-Eu1-O7	78.6(2)
Eu1-O7	2.400(5)	O1-Eu1-N1	72.9(2)
Eu1-N1	2.632(6)	O1-Eu1-N2	119.0(2)
Eu1-N2	2.576(6)	O3#1-Eu1-O4#1	51.94(17)
O5-Eu1-N2	83.0(2)	O3#1-Eu1-N1	70.4(2)
O6#2-Eu1-O3#1	150.95(19)	O3#1-Eu1-N2	79.48(19)
O6#2-Eu1-O4#1	156.18(19)	O4#1-Eu1-N1	81.31(19)
O6#2-Eu1-O7	85.18(18)	O4#1-Eu1-N2	127.38(19)
O6#2-Eu1-N1	110.05(19)	O5-Eu1-O3#1	75.71(19)
O6#2-Eu1-N2	75.8(2)	O5-Eu1-O4#1	100.70(18)
O7-Eu1-O3#1	111.11(18)	O5-Eu1-O6#2	86.21(19)
O7-Eu1-O4#1	74.85(17)	O5-Eu1-O7	75.04(19)
O7-Eu1-N1	145.52(19)	O5-Eu1-N1	134.7(2)
O7-Eu1-N2	151.80(18)	N2-Eu1-N1	62.20(19)

Symmetry codes #1: +X,1-Y,-1/2+Z; #2: 1-X,+Y,3/2-Z; #3: -X,+Y,3/2-Z; #4: +X,1+Y,+Z; #5: -X,1+Y,3/2-Z; #6: +X,2-Y,1/2+Z; #7: -X,2-Y,1-Z; #8: +X,1-Y,1/2+Z; #9: +X,-1+Y,+Z.

#### DZU-500(Eu)⊂Pyrene(423K)

Eu1-O1	2.353(3)	O1-Eu1-O2#1	86.80(11)
Eu1-O2#1	2.362(3)	O1-Eu1-O5#2	75.61(12)
Eu1-O3	2.281(3)	O1-Eu1-O6#2	100.34(11)
Eu1-O5#2	2.480(3)	O1-Eu1-O7	75.66(11)
Eu1-O6#2	2.489(3)	O1-Eu1-N1	82.44(11)
Eu1-O7	2.400(3)	O1-Eu1-N2	134.49(11)
Eu1-N1	2.587(3)	O2#1-Eu-O5#2	151.39(11)
Eu1-N2	2.621(4)	O2#1-Eu1-O6#2	155.90(11)
O3-Eu1-O7	78.05(12)	O2#1-Eu1-O7	85.14(11)
O3-Eu1-N1	119.63(12)	O2#1-Eu1-N1	76.28(11)
O3-Eu1-N2	72.79(12)	O2#1-Eu1-N2	109.90(12)
O5#2-Eu1-O6#2	51.84(10)	O3-Eu1-O1	152.66(13)
O5#2-Eu1-N1	79.14(11)	O3-Eu1-O2#1	83.61(12)
O5#2-Eu1-N2	70.27(12)	O3-Eu1-O5#2	121.72(12)
O6#2-Eu1-N1	127.26(11)	O3-Eu1-O6#2	79.61(11)

O6#2-Eu1-N2	81.48(11)	O7-Eu1-N1	151.98(11)
O7-Eu1-O5#2	111.34(11)	O7-Eu1-N2	145.06(13)
O7-Eu1-O6#2	74.59(10)	N1-Eu1-N2	62.51(11)

Symmetry codes #1: 1-X,1-Y,-Z; #2: X,-1+Y,Z; #3: 1-X,-Y, -Z; #4: 1-X,-Y,1-Z;

#### **DZU-500(Gd)⊂Pyrene**

Gd1-N1	2.555(3)	O(1)-Gd(1)-O(2)#1	86.61(10)
Gd1-N2	2.590(3)	O(1)-Gd(1)-O(5)#2	75.37(10)
Gd1-O1	2.338(3)	O(1)-Gd(1)-O(6)#2	100.33(10)
Gd1-O2#1	2.340(3)	O(1)-Gd(1)-O(7)	75.27(10)
Gd1-O3	2.276(3)	O(1)-Gd(1)-N(1)	81.92(10)
Gd1-O5#2	2.490(3)	O(1)-Gd(1)-N(2)	134.35(10)
Gd1-O6#2	2.458(3)	O(2)#1-Gd(1)-O(5)#2	150.80(10)
Gd1-O7	2.375(3)	O(2)#1-Gd(1)-O(6)#2	155.40(10)
O(5)#2-Gd(1)-N(2)	69.74(10)	O(2)#1-Gd(1)-O(7)	84.73(10)
O(6)#2-Gd(1)-O(5)#2	52.83(9)	O(2)#1-Gd(1)-N(1)	75.98(10)
O(6)#2-Gd(1)-N(1)	128.16(10)	O(2)#1-Gd(1)-N(2)	110.69(10)
O(6)#2-Gd(1)-N(2)	81.29(10)	O(3)-Gd(1)-O(1)	152.65(11)
O(7)-Gd(1)-O(5)#2	111.80(9)	O(3)-Gd(1)-O(2)#1	83.05(10)
O(7)-Gd(1)-O(6)#2	74.47(9)	O(3)-Gd(1)-O(5)#2	122.75(10)
O(7)-Gd(1)-N(1)	150.88(10)	O(3)-Gd(1)-O(6)#2	80.13(10)
O(7)-Gd(1)-N(2)	145.27(10)	O(3)-Gd(1)-O(7)	78.62(10)
N(1)-Gd(1)-N(2)	63.44(10)	O(3)-Gd(1)-N(1)	119.55(11)
O(5)#2-Gd(1)-N(1)	78.84(10)	O(3)-Gd(1)-N(2)	72.96(11)

Symmetry codes #1: 1-X,2-Y,2-Z; #2: X,-1+Y,Z; #3: X,1+Y, Z; #4: 1-X,1-Y,2-Z; #5: 1-X,2-Y,1-Z;

#### **DZU-500(Sm)⊂Pyrene**

N1-Sm1	2.588(4)	O(1)-Sm(1)-O(5)#1	151.28(11)
N2-Sm1	2.621(4)	O(1)-Sm(1)-O(6)#1	155.70(11)
O1-Sm1	2.360(3)	O(1)-Sm(1)-O(7)	84.77(11)
O2#1-Sm1	2.359(4)	O(1)-Sm(1)-N(1)	75.94(12)
O3-Sm1	2.301(3)	O(1)-Sm(1)-N(2)	110.47(12)
O5#2-Sm1	2.514(3)	O(2)#2-Sm(1)-O(1)	86.35(12)
O6#2-Sm1	2.486(3)	O(2)#2-Sm(1)-O(5)#1	75.85(12)
O7-Sm1	2.398(3)	O(2)#2-Sm(1)-O(6)#1	100.84(11)
O(6)#1-Sm(1)-O(5)#1	52.14(10)	O(2)#2-Sm(1)-O(7)	75.61(12)
O(6)#1-Sm(1)-N(1)	127.84(11)	O(2)#2-Sm(1)-N(1)	81.71(12)
O(6)#1-Sm(1)-N(2)	81.35(12)	O(2)#2-Sm(1)-N(2)	133.69(12)
O(7)-Sm(1)-O(5)#1	111.63(11)	O(3)-Sm(1)-O(1)	83.91(12)

O(7)-Sm(1)-O(6)#1	74.80(11)	O(3)-Sm(1)-O(2)#2	153.33(13)
O(7)-Sm(1)-N(1)	151.03(12)	O(3)-Sm(1)-O(5)#1	121.41(12)
O(7)-Sm(1)-N(2)	145.82(12)	O(3)-Sm(1)-O(6)#1	79.39(11)
N(1)-Sm(1)-N(2)	62.72(12)	O(3)-Sm(1)-O(7)	78.81(13)
O(5)#1-Sm(1)-N(1)	79.28(11)	O(3)-Sm(1)-N(1)	119.51(13)
O(5)#1-Sm(1)-N(2)	69.48(13)	O(3)-Sm(1)-N(2)	72.94(13)

Symmetry codes #1: 1-X,1-Y,-Z; #2: X,1+Y,Z; #3: 1-X,-Y,-Z; #4: X,-1+Y,Z; #5: 1-X,-Y,1-Z;

### DZU-500(Tb)⊂Pyrene

N1-Tb1	2.543(4)	O(1)-Tb(1)-N(1)	78.35(12)
N2-Tb1	2.587(5)	O(1)-Tb(1)-N(2)	70.08(13)
O1-Tb1	2.474(3)	O(2)-Tb(1)-O(1)	52.90(11)
O2-Tb1	2.453(3)	O(2)-Tb(1)-N(1)	127.59(12)
O3#1-Tb1	2.268(3)	O(2)-Tb(1)-N(2)	80.87(12)
O5-Tb1	2.327(3)	O(3)#1-Tb(1)-O(1)	123.00(12)
O6#2-Tb1	2.328(4)	O(3)#1-Tb(1)-O(2)	79.77(12)
O7-Tb1	2.361(3)	O(3)#1-Tb(1)-O(5)	83.30(12)
O(6)#2-Tb(1)-O(2)	100.71(12)	O(3)#1-Tb(1)-O(6)#2	152.25(13)
O(6)#2-Tb(1)-O(7)	75.25(12)	O(3)#1-Tb(1)-O(7)	78.18(13)
O(6)#2-Tb(1)-N(1)	81.69(13)	O(3)#1-Tb(1)-N(1)	120.29(13)
O(6)#2-Tb(1)-N(2)	134.66(12)	O(3)#1-Tb(1)-N(2)	73.05(13)
O(7)-Tb(1)-O(1)	111.86(12)	O(5)-Tb(1)-O(1)	150.38(12)
O(7)-Tb(1)-O(2)	74.89(11)	O(5)-Tb(1)-O(2)	155.84(12)
O(7)-Tb(1)-N(1)	150.88(12)	O(5)-Tb(1)-O(6)#2	86.47(12)
O(7)-Tb(1)-N(2)	145.11(12)	O(5)-Tb(1)-O(7)	84.90(12)
N(1)-Tb(1)-N(2)	63.62(12)	O(5)-Tb(1)-N(1)	76.06(12)
O(6)#2-Tb(1)-O(1)	75.24(12)	O(5)-Tb(1)-N(2)	110.47(13)

Symmetry codes #1: 1-X,2-Y,2-Z; #2: X,-1+Y,Z; #3: 1-X,1-Y,2-Z; #4: X,1+Y,Z; #5: 1-X,2-Y,1-Z;