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Electronic Supplementary Information

Mixed (Phthalocyanine)(Schiff-Base) Terbium(III)-Alkali Metal(I)/Zinc(II) Complexes. Synthesis, Structures, and Spectroscopic Properties

Qi Ma, Xuenan Feng, Wei Cao, Hailong Wang, and Jianzhuang Jiang*

Fig. S1. Molecular structures of **2**, **4**, and **5** in side view with all hydrogen atoms omitted for clarity and the ellipsoids drawn at the 30% probability level.

Fig. S2. Packing plots of **1**, **2**, **3**, **4**, and **5**.

Fig. S3. The electronic absorption spectra of **1**, **2**, **3**, **4**, and **5** in a mixed solvent of MeOH/THF (1:9) with ZnL and Tb(Pc)(acac) as references.

Fig. S4. The luminescence spectra of Li(Pc)Tb(L)$(CH_3OH)_2$·THF (**1**), M(Pc)Tb(L)(CH_3OH) (M = Na, K, Rb, Cs) (**2-5**), in a mixed solvent of MeOH/THF (1:9) at the concentration of 4×10^{-6} M with an excitation wavelength of 330 nm together with ZnL and Tb(Pc)(acac) as references.

Fig. S5. The luminescence spectra of titrating Zn(II) into Li(Pc)Tb(L)$(CH_3OH)_2$ (**1**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4×10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm.

Fig. S6. The luminescence spectra of titrating Zn(II) into Na(Pc)Tb(L)(CH_3OH) (**2**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4×10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm.

Fig. S7. The luminescence spectra of titrating Zn(II) into Rb(Pc)Tb(L)(CH_3OH) (**4**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4×10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm..

Fig. S8. The luminescence spectra of titrating Zn(II) into Cs(Pc)Tb(L)(CH_3OH) (**5**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4×10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm.

Fig. S9. Packing plot of **6**.

Fig. S10. XRPD diffraction patterns of **1**, **2**, **3**, **4**, and **5** (black line) together with those simulated from single crystal XRD data (red line).

Table S1. Selected bond distances (Å) and bond angles (o) of **1-6**.

Table S2. Analytical and mass spectroscopic data for the series of sandwich-type complexes **1-6** and complexes **1-5** with Zn (II).

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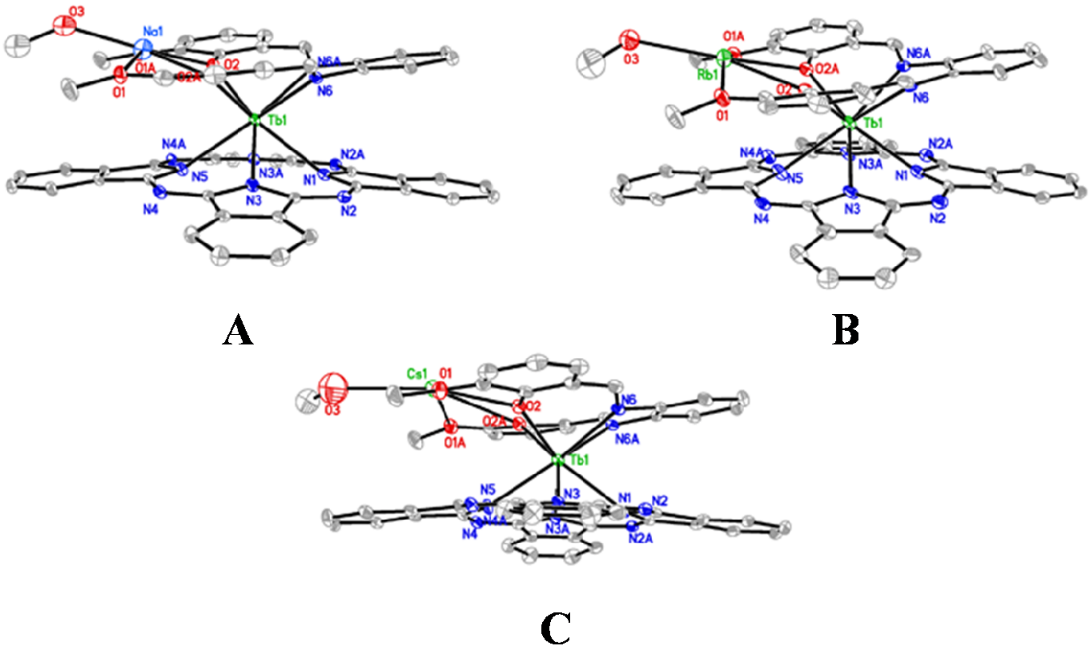

Fig. S1. Molecular structures of **2** (A), **4** (B), and **5** (C) in side view with all hydrogen atoms omitted for clarity and the ellipsoids drawn at the 30% probability level. The symmetry codes are a) x, y, -z-1/2; b) x-1, y, z; c) x+1, y, z; d) x+1, y, -z-1/2 for **4** and a) x, y, -z-1/2; b) x-1, y, z; c) x+1 ,y ,z; d) x+1, y,-z-1/2 for **5**.

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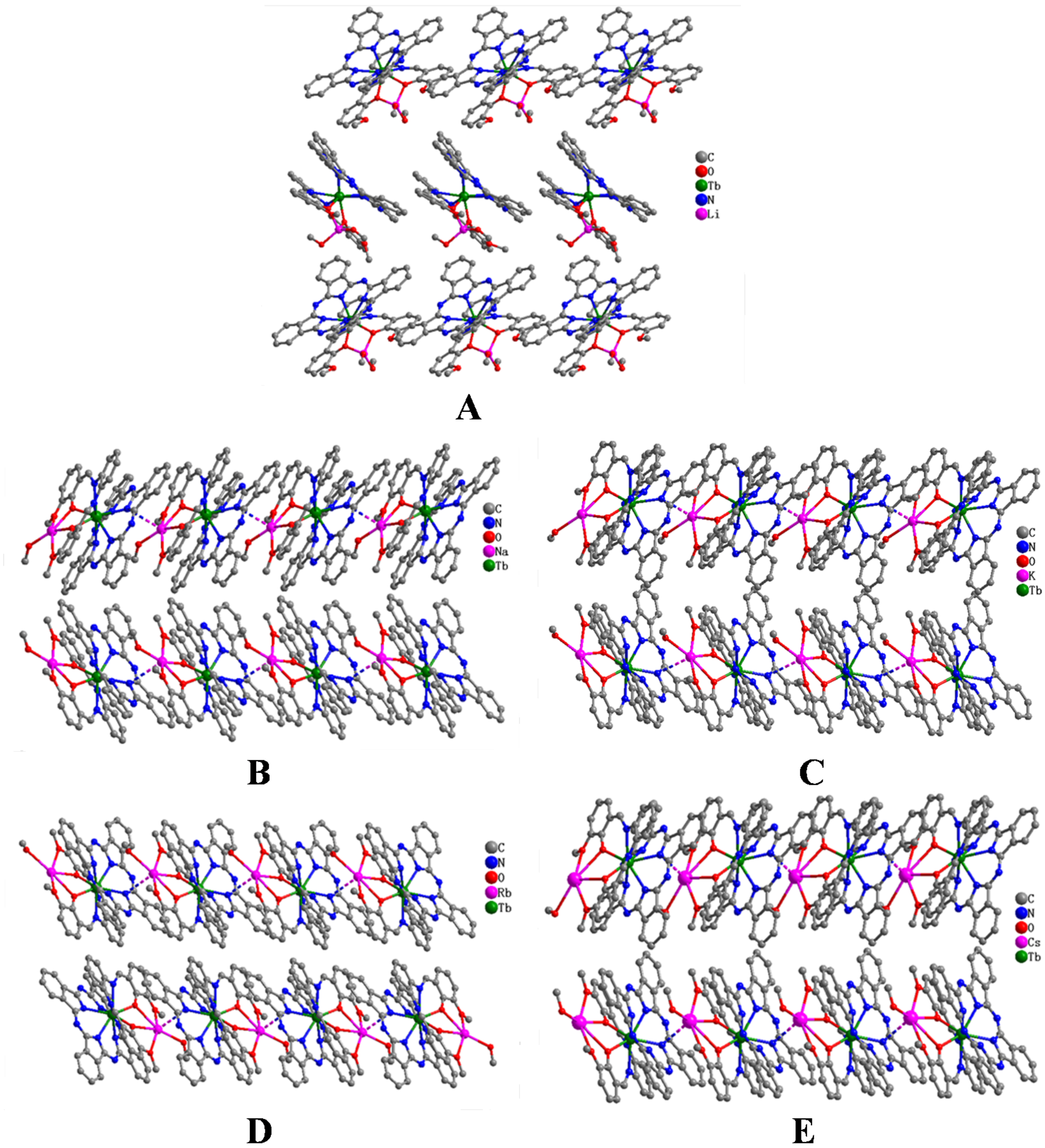

Fig. S2. Packing plots of **1** (A), **2** (B), **3** (C), **4** (D), and **5** (E).

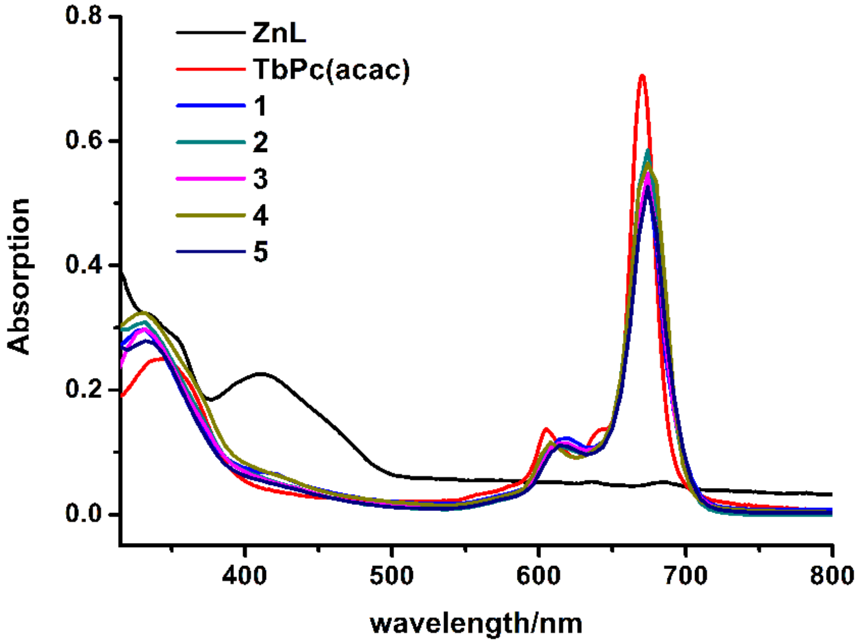

Fig. S3. The electronic absorption spectra of **1**, **2**, **3**, **4**, and **5** in a mixed solvent of MeOH/THF (1:9) with ZnL and Tb(Pc)(acac) as references.

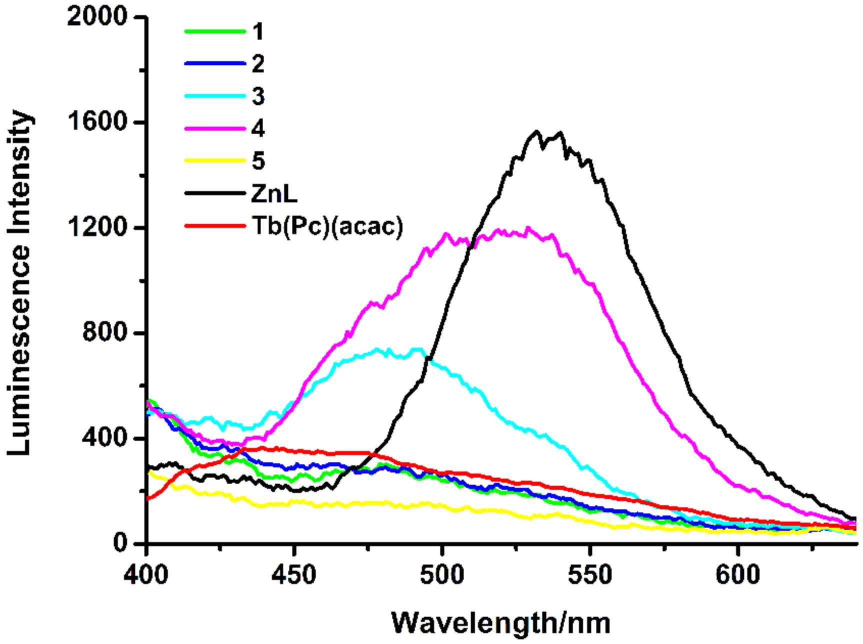

Fig. S4. The luminescence spectra of Li(Pc)Tb(L)$(CH_3OH)_2$·THF (**1**), M(Pc)Tb(L)(CH_3OH) (M = Na, K, Rb, Cs) (**2**-**5**), in a mixed solvent of MeOH/THF (1:9) at the concentration of 4 × 10^{-6} M with an excitation wavelength of 330 nm together with ZnL and Tb(Pc)(acac) as references.

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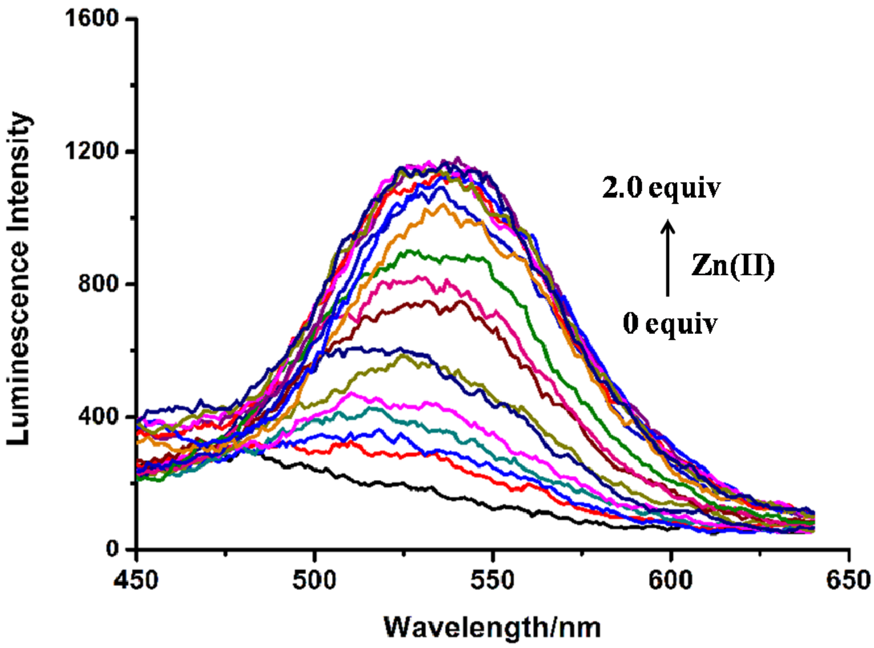

Fig. S5. The luminescence spectra of titrating Zn(II) into Li(Pc)Tb(L)$(CH_3OH)_2$ (**1**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4 × 10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm.

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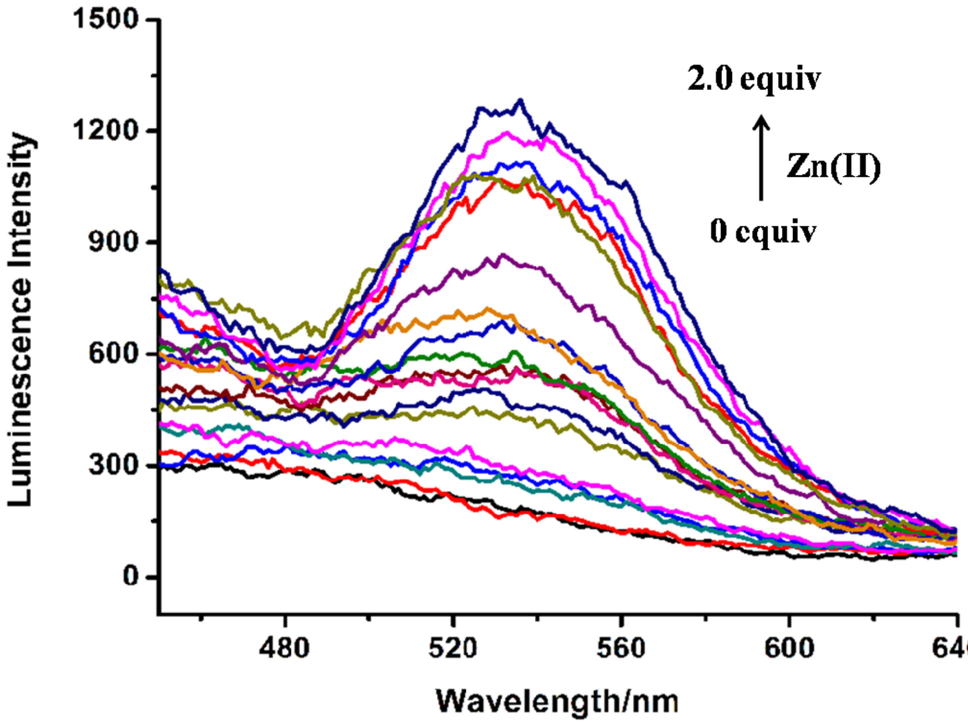

Fig. S6. The luminescence spectra of titrating Zn(II) into Na(Pc)Tb(L)(CH_3OH) (**2**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4 × 10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm.

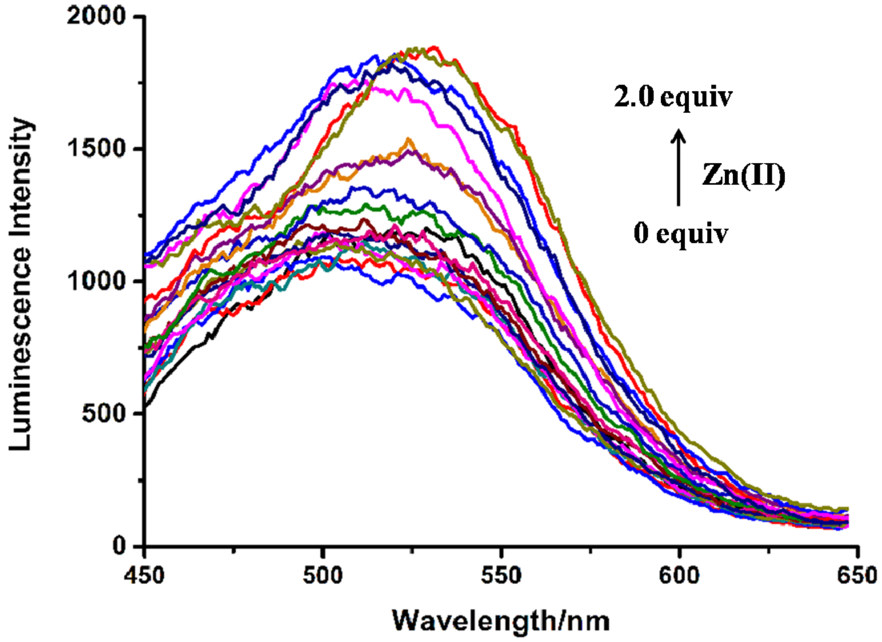

Fig. S7. The luminescence spectra of titrating Zn(II) into Rb(Pc)Tb(L)(CH_3OH) (**4**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4 × 10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm.

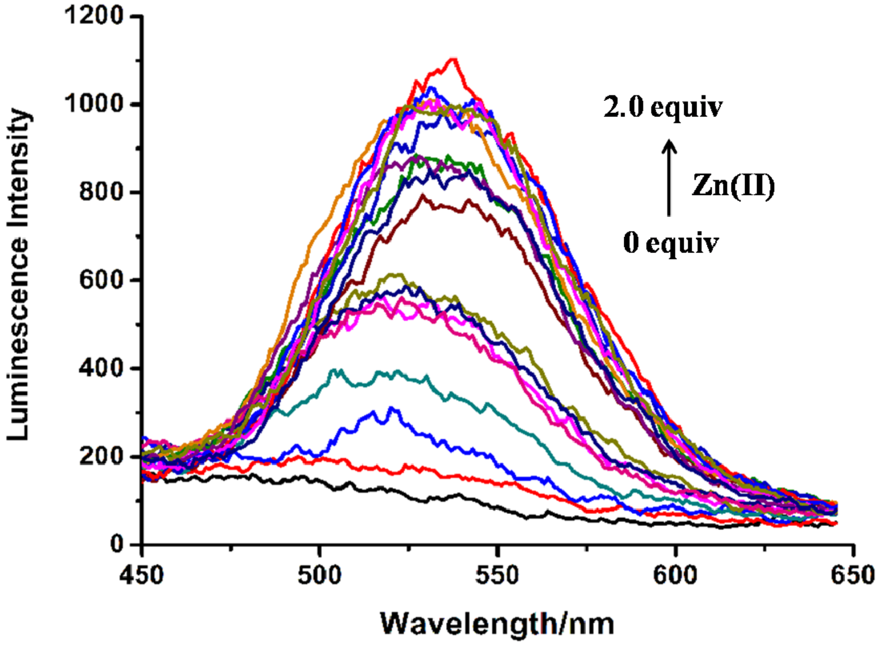

Fig. S8. The luminescence spectra of titrating Zn(II) into Cs(Pc)Tb(L)(CH_3OH) (**5**) in a mixed solvent of MeOH/THF (1:9) at the concentration of 4×10^{-6} M with increasing amount of Zn(II) (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2. 1.5, 1.6, 1.8, 1.9, and 2.0 equiv) with an excitation wavelength of 330 nm.

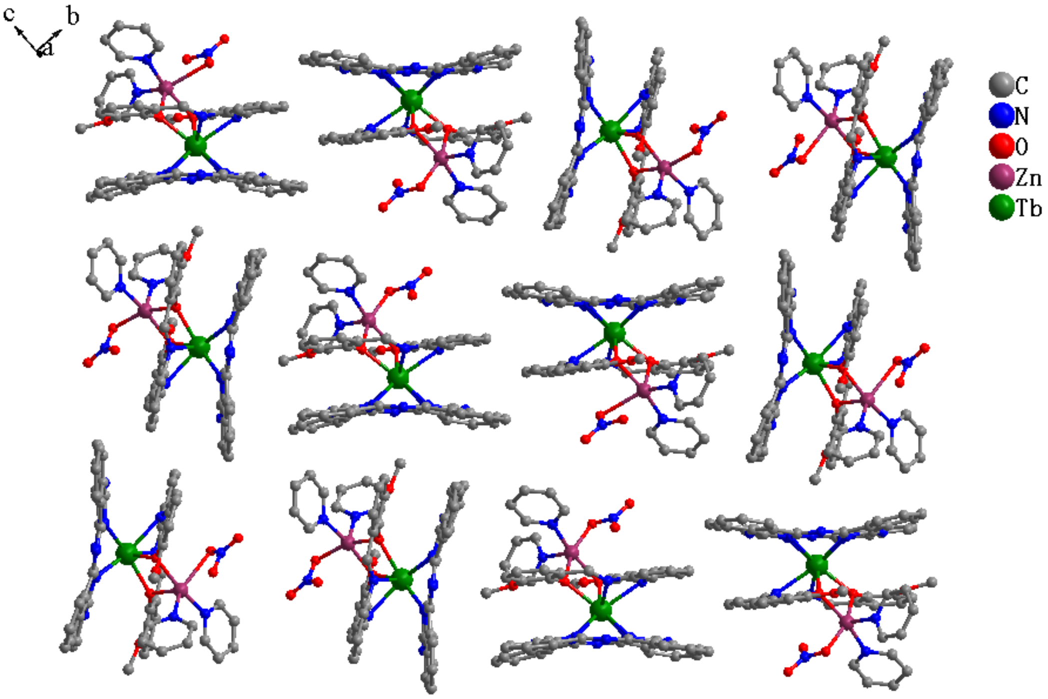

Fig. S9. Packing plot of **6**.

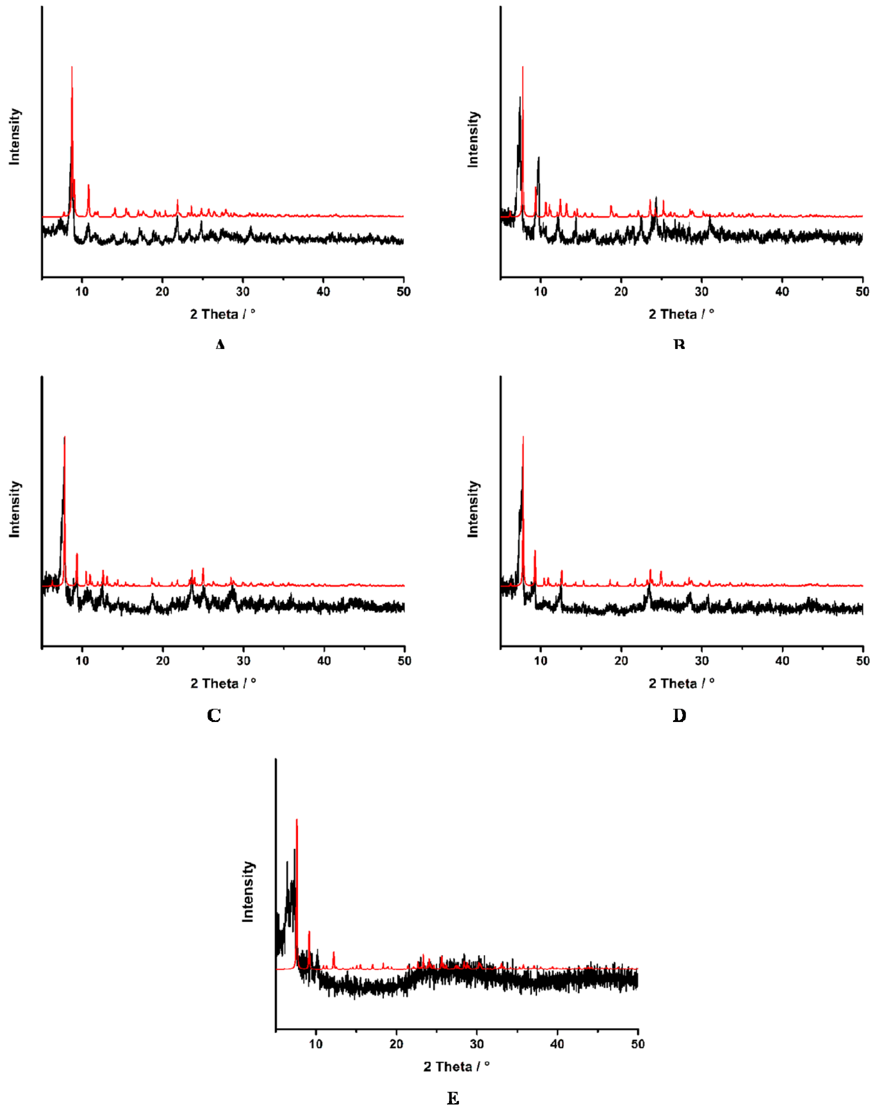

Fig. S10. XRPD diffraction patterns of **1**, **2**, **3**, **4**, and **5** (black line) together with those simulated from single crystal XRD data (red line).

Table S1 Selected bond distances (Å) and bond angles (°) of **1-6**.

Complex **1**			
O(2)-Li(1)	2.051(13)	Tb(01)-N(3)	2.420(4)
O(2)-Tb(01)	2.289(3)	Tb(01)-N(5)	2.434(4)
O(3)-Li(1)	2.000(13)	Tb(01)-N(1)	2.436(4)
O(3)-Tb(01)	2.290(4)	b(01)-N(7)	2.438(4)
O(5)-Li(1)	2.040(15)	Tb(01)-N(10)	2.510(4)
O(6)-Li(1)	1.794(18)	Tb(01)-N(9)	2.521(4)
O(6A)-Li(1)	1.83(2)		
O(2)-Tb(01)-O(3)	73.56(13)	O(6)-Li(1)-O(6A)	34.0(6)
O(2)-Tb(01)-N(3)	81.82(13)	O(6)-Li(1)-O(3)	118.5(8)
O(3)-Tb(01)-N(3)	147.47(14)	O(6A)-Li(1)-O(3)	129.8(9)
O(2)-Tb(01)-N(5)	142.13(13)	O(6)-Li(1)-O(5)	131.8(8)
O(3)-Tb(01)-N(5)	140.91(13)	O(6A)-Li(1)-O(5)	99.5(8)
N(3)-Tb(01)-N(5)	70.01(13)	O(3)-Li(1)-O(5)	101.4(7)
O(2)-Tb(01)-N(1)	84.56(13)	O(6)-Li(1)-O(2)	104.5(8)
O(3)-Tb(01)-N(1)	85.29(14)	O(6A)-Li(1)-O(2)	131.7(9)
N(3)-Tb(01)-N(1)	71.29(14)	O(3)-Li(1)-O(2)	85.2(5)
N(5)-Tb(01)-N(1)	108.55(14)	O(5)-Li(1)-O(2)	104.8(7)
O(2)-Tb(01)-N(7)	145.45(14)	O(6)-Li(1)-Tb(01)	109.2(6)
O(3)-Tb(01)-N(7)	81.28(14)	O(6A)-Li(1)-Tb(01)	141.9(8)
N(3)-Tb(01)-N(7)	109.95(14)	O(3)-Li(1)-Tb(01)	43.5(3)
N(5)-Tb(01)-N(7)	70.47(14)	O(5)-Li(1)-Tb(01)	118.5(6)
N(1)-Tb(01)-N(7)	69.91(14)	O(2)-Li(1)-Tb(01)	43.7(3)
O(2)-Tb(01)-N(10)	109.79(13)	N(3)-Tb(01)-N(9)	83.21(13)
O(3)-Tb(01)-N(10)	72.45(14)	N(5)-Tb(01)-N(9)	79.28(13)
N(3)-Tb(01)-N(10)	137.40(14)	N(1)-Tb(01)-N(9)	147.92(13)
N(5)-Tb(01)-N(10)	78.05(13)	N(7)-Tb(01)-N(9)	139.36(14)
N(1)-Tb(01)-N(10)	147.97(13)	N(10)-Tb(01)-N(9)	63.35(13)
N(7)-Tb(01)-N(10)	83.90(13)	O(3)-Tb(01)-N(9)	108.50(13)
O(2)-Tb(01)-N(9)	72.55(13)		
Complex **2**			
N(1)-Tb(1)	2.450(4)	O(3)-Na(1)	2.236(5)
N(3)-Tb(1)	2.447(3)	Na(1)-O(2)#1	2.360(3)
N(5)-Tb(1)	2.453(4)	Na(1)-O(1)#1	2.785(3)
N(6)-Tb(1)	2.484(2)	Tb(1)-O(2)#1	2.264(2)
O(2)-Tb(1)	2.264(2)	Tb(1)-N(3)#1	2.447(3)
O(2)-Na(1)	2.360(3)	Tb(1)-N(6)#1	2.484(2)
O(3)-Na(1)-O(2)	144.93(6)	N(3)-Tb(1)-N(6)#1	139.56(8)
O(3)-Na(1)-O(2)#1	144.93(6)	N(1)-Tb(1)-N(6)#1	79.67(9)

O(2)-Na(1)-O(2)#1	70.12(12)	N(5)-Tb(1)-N(6)#1	147.15(6)
O(3)-Na(1)-O(1)#1	85.35(7)	O(2)-Tb(1)-N(6)	72.90(8)
O(2)-Na(1)-O(1)#1	128.89(11)	O(2)#1-Tb(1)-N(6)	110.52(8)
O(2)#1-Na(1)-O(1)#1	59.98(7)	N(3)#1-Tb(1)-N(6)	139.56(8)
O(3)-Na(1)-O(1)	85.35(7)	N(3)-Tb(1)-N(6)	83.87(8)
O(2)-Na(1)-O(1)	59.98(7)	N(1)-Tb(1)-N(6)	79.67(9)
O(2)#1-Na(1)-O(1)	128.89(11)	N(5)-Tb(1)-N(6)	147.15(6)
O(1)#1-Na(1)-O(1)	158.23(14)	N(6)#1-Tb(1)-N(6)	65.11(11)
O(2)-Tb(1)-O(2)#1	73.59(11)	O(2)-Tb(1)-Na(1)	39.64(6)
O(2)-Tb(1)-N(3)#1	145.79(8)	O(2)#1-Tb(1)-Na(1)	39.64(6)
O(2)#1-Tb(1)-N(3)#1	82.01(8)	N(3)#1-Tb(1)-Na(1)	107.56(6)
O(2)-Tb(1)-N(3)	82.01(8)	N(3)-Tb(1)-Na(1)	107.56(6)
O(2)#1-Tb(1)-N(3)	145.79(8)	N(1)-Tb(1)-Na(1)	173.98(9)
N(3)#1-Tb(1)-N(3)	107.51(12)	N(5)-Tb(1)-Na(1)	67.01(9)
O(2)-Tb(1)-N(1)	142.08(6)	N(6)#1-Tb(1)-Na(1)	105.35(7)
O(2)#1-Tb(1)-N(1)	142.08(6)	N(6)-Tb(1)-Na(1)	105.35(7)
N(3)#1-Tb(1)-N(1)	69.31(7)	N(3)-Tb(1)-N(5)	69.49(7)
N(3)-Tb(1)-N(1)	69.31(7)	N(1)-Tb(1)-N(5)	106.98(12)
O(2)-Tb(1)-N(5)	84.33(9)	O(2)-Tb(1)-N(6)#1	110.52(8)
O(2)#1-Tb(1)-N(5)	84.33(9)	O(2)#1-Tb(1)-N(6)#1	72.90(8)
N(3)#1-Tb(1)-N(5)	69.49(7)	N(3)#1-Tb(1)-N(6)#1	83.87(8)

Complex **3**

N(1)-Tb(1)	2.445(5)	Tb(1)-N(6)#1	2.485(4)
N(3)-Tb(1)	2.453(4)	K(1)-O(1)#1	2.828(3)
N(5)-Tb(1)	2.454(5)	K(1)-N(1)#3	3.162(5)
N(6)-Tb(1)	2.485(4)	K(1)-O(3)#1	2.660(7)
O(1)-K(1)	2.828(3)	K(1)-O(2)#1	2.630(3)
O(2)-Tb(1)	2.262(3)	Tb(1)-O(2)#1	2.262(3)
O(2)-K(1)	2.630(3)	Tb(1)-N(3)#1	2.453(4)
O(3)-K(1)	2.660(7)		

O(2)#1-K(1)-O(2)	63.97(13)	N(1)-Tb(1)-N(3)#1	69.21(11)
O(2)#1-K(1)-O(3)#1	156.24(17)	O(2)-Tb(1)-N(3)	80.92(12)
O(2)-K(1)-O(3)#1	138.82(17)	O(2)#1-Tb(1)-N(3)	146.24(12)
O(2)#1-K(1)-O(3)	138.82(17)	N(1)-Tb(1)-N(3)	69.21(11)
O(2)-K(1)-O(3)	156.24(17)	N(3)#1-Tb(1)-N(3)	106.82(18)
O(3)#1-K(1)-O(3)	17.7(3)	O(2)-Tb(1)-N(5)	83.85(13)
O(2)#1-K(1)-O(1)	120.07(10)	O(2)#1-Tb(1)-N(5)	83.85(13)
O(2)-K(1)-O(1)	57.04(9)	N(1)-Tb(1)-N(5)	107.09(17)
O(3)#1-K(1)-O(1)	81.81(17)	N(3)#1-Tb(1)-N(5)	69.31(11)
O(3)-K(1)-O(1)	99.24(17)	N(3)-Tb(1)-N(5)	69.31(11)
O(2)#1-K(1)-O(1)#1	57.04(9)	O(2)-Tb(1)-N(6)#1	111.69(12)
O(2)-K(1)-O(1)#1	120.07(10)	O(2)#1-Tb(1)-N(6)#1	72.77(12)

O(3)#1-K(1)-O(1)#1	99.24(17)	N(1)-Tb(1)-N(6)#1	79.55(13)
O(3)-K(1)-O(1)#1	81.81(17)	N(3)#1-Tb(1)-N(6)#1	83.98(12)
O(1)-K(1)-O(1)#1	161.20(15)	N(3)-Tb(1)-N(6)#1	139.73(13)
O(2)-Tb(1)-O(2)#1	76.04(15)	N(5)-Tb(1)-N(6)#1	146.99(9)
O(2)-Tb(1)-N(1)	141.03(8)	O(2)-Tb(1)-N(6)	72.77(12)
O(2)#1-Tb(1)-N(1)	141.03(8)	O(2)#1-Tb(1)-N(6)	111.69(12)
O(2)-Tb(1)-N(3)#1	146.24(12)	N(1)-Tb(1)-N(6)	79.55(13)
O(2)#1-Tb(1)-N(3)#1	80.92(12)	N(3)#1-Tb(1)-N(6)	139.73(13)
N(6)#1-Tb(1)-N(6)	65.43(17)	N(3)-Tb(1)-N(6)	83.98(12)

Complex **4**

N(1)-Tb(1)	2.442(9)	Rb(1)-O(3)#1	2.815(11)
N(1)-Rb(1)#2	3.194(8)	Rb(1)-O(1)#1	2.910(4)
N(3)-Tb(1)	2.454(5)	Rb(1)-N(1)#3	3.194(8)
O(3)-Rb(1)	2.815(11)	Rb(1)-O(2)#1	2.768(4)
N(5)-Tb(1)	2.462(7)	Tb(1)-N(6)#1	2.497(5)
N(5)-Rb(1)	3.669(9)	O(2)-Rb(1)	2.768(4)
N(6)-Tb(1)	2.497(5)	Rb(1)-H(3A)	2.2714
O(1)-Rb(1)	2.910(4)	Tb(1)-O(2)#1	2.257(4)
O(2)-Tb(1)	2.257(4)	Tb(1)-N(3)#1	2.454(5)

O(2)#1-Rb(1)-O(3)#1	161.0(2)	O(2)#1-Rb(1)-O(2)	61.57(16)
O(2)-Rb(1)-O(3)#1	136.1(2)	N(5)-Tb(1)-N(6)	147.42(11)
O(2)#1-Rb(1)-O(3)	136.1(2)	O(2)#1-Rb(1)-N(5)	56.71(13)
O(2)-Rb(1)-O(3)	161.0(2)	O(2)-Rb(1)-N(5)	56.71(13)
O(3)#1-Rb(1)-O(3)	25.4(4)	O(3)#1-Rb(1)-N(5)	122.4(3)
O(2)#1-Rb(1)-O(1)#1	55.06(13)	O(3)-Rb(1)-N(5)	122.4(3)
O(2)-Rb(1)-O(1)#1	115.90(13)	O(1)#1-Rb(1)-N(5)	80.64(10)
O(3)#1-Rb(1)-O(1)#1	106.1(2)	O(1)-Rb(1)-N(5)	80.64(10)
O(3)-Rb(1)-O(1)#1	81.0(2)	N(1)#3-Rb(1)-N(5)	153.69(19)
O(2)#1-Rb(1)-O(1)	115.90(13)	C(4)#4-Rb(1)-N(5)	135.69(16)
O(2)-Rb(1)-O(1)	55.06(13)	C(4)#3-Rb(1)-N(5)	135.69(16)
O(3)#1-Rb(1)-O(1)	81.0(2)	O(2)-Tb(1)-O(2)#1	77.7(2)
O(3)-Rb(1)-O(1)	106.1(2)	O(2)-Tb(1)-N(1)	140.16(11)
O(1)#1-Rb(1)-O(1)	160.9(2)	O(2)#1-Tb(1)-N(1)	140.16(11)
O(2)#1-Rb(1)-N(1)#3	101.48(16)	O(2)-Tb(1)-N(3)#1	146.87(18)
O(2)-Rb(1)-N(1)#3	101.48(16)	O(2)#1-Tb(1)-N(3)#1	80.10(17)
O(3)#1-Rb(1)-N(1)#3	83.1(3)	N(1)-Tb(1)-N(3)#1	69.31(17)
O(3)-Rb(1)-N(1)#3	83.1(3)	O(2)-Tb(1)-N(3)	80.10(17)
O(1)#1-Rb(1)-N(1)#3	99.21(10)	O(2)#1-Tb(1)-N(3)	146.87(18)
O(1)-Rb(1)-N(1)#3	99.21(10)	N(1)-Tb(1)-N(3)	69.31(17)
N(1)-Tb(1)-N(6)#1	79.0(2)	N(3)#1-Tb(1)-N(3)	107.1(3)
N(3)#1-Tb(1)-N(6)#1	84.01(17)	O(2)-Tb(1)-N(5)	83.89(19)
N(3)-Tb(1)-N(6)#1	139.09(18)	O(2)#1-Tb(1)-N(5)	83.89(19)

N(5)-Tb(1)-N(6)#1	147.42(11)	N(1)-Tb(1)-N(5)	107.4(3)
O(2)-Tb(1)-N(6)	72.88(17)	N(3)#1-Tb(1)-N(5)	69.47(17)
O(2)#1-Tb(1)-N(6)	112.14(16)	N(3)-Tb(1)-N(5)	69.47(17)
O(2)#1-Tb(1)-N(6)#1	72.88(17)	O(2)-Tb(1)-N(6)#1	112.14(16)

Complex **5**

N(1)-Tb(1)	2.447(7)	Cs(1)-O(2)#1	2.996(4)
N(1)-Cs(1)#2	3.194(7)	Cs(1)-O(1)#1	3.030(4)
N(3)-Tb(1)	2.463(5)	Cs(1)-O(3)	3.031(19)
N(3)-Cs(1)#2	3.763(5)	Cs(1)-O(3)#1	3.031(19)
Tb(1)-N(6)#1	2.502(5)	Cs(1)-N(1)#3	3.194(7)
N(5)-Tb(1)	2.474(6)	O(2)-Cs(1)	2.996(4)
N(5)-Cs(1)	3.848(7)	Tb(1)-N(3)#1	2.463(5)
N(6)-Tb(1)	2.502(5)	Cs(1)-N(3)#3	3.763(5)
O(1)-Cs(1)	3.030(4)	Cs(1)-N(3)#4	3.763(5)
O(2)-Tb(1)	2.270(4)	Tb(1)-O(2)#1	2.270(4)

O(2)#1-Cs(1)-O(2)	57.72(15)	O(2)-Tb(1)-O(2)#1	79.2(2)
O(2)#1-Cs(1)-O(1)	108.53(11)	O(2)-Tb(1)-N(1)	139.13(11)
O(2)-Cs(1)-O(1)	51.68(11)	O(2)#1-Tb(1)-N(1)	139.13(11)
O(2)#1-Cs(1)-O(1)#1	51.68(11)	O(2)-Tb(1)-N(3)#1	148.31(15)
O(2)-Cs(1)-O(1)#1	108.53(11)	O(2)#1-Tb(1)-N(3)#1	80.51(15)
O(1)-Cs(1)-O(1)#1	152.60(17)	N(1)-Tb(1)-N(3)#1	69.03(14)
O(2)#1-Cs(1)-O(3)	158.7(4)	O(2)-Tb(1)-N(3)	80.51(15)
O(2)-Cs(1)-O(3)	125.4(3)	O(2)#1-Tb(1)-N(3)	148.31(15)
O(1)-Cs(1)-O(3)	74.8(3)	N(1)-Tb(1)-N(3)	69.03(14)
O(1)#1-Cs(1)-O(3)	116.5(3)	N(3)#1-Tb(1)-N(3)	105.7(2)
O(2)#1-Cs(1)-O(3)#1	125.4(3)	O(2)-Tb(1)-N(5)	84.72(16)
O(2)-Cs(1)-O(3)#1	158.7(4)	O(2)#1-Tb(1)-N(5)	84.72(16)
O(1)-Cs(1)-O(3)#1	116.5(3)	N(1)-Tb(1)-N(5)	108.0(2)
O(1)#1-Cs(1)-O(3)#1	74.8(3)	N(3)#1-Tb(1)-N(5)	69.39(14)
O(3)-Cs(1)-O(3)#1	42.8(5)	N(3)-Tb(1)-N(5)	69.39(14)
O(2)#1-Tb(1)-N(6)	112.61(14)	O(2)-Tb(1)-N(6)#1	112.61(14)
N(1)-Tb(1)-N(6)	77.42(17)	O(2)#1-Tb(1)-N(6)#1	72.66(14)
N(3)#1-Tb(1)-N(6)	138.23(16)	N(1)-Tb(1)-N(6)#1	77.42(17)
N(3)-Tb(1)-N(6)	83.79(15)	N(3)#1-Tb(1)-N(6)#1	83.79(15)
N(5)-Tb(1)-N(6)	147.49(11)	N(3)-Tb(1)-N(6)#1	138.23(15)
N(6)#1-Tb(1)-N(6)	64.8(2)	N(5)-Tb(1)-N(6)#1	147.49(11)

Complex **6**

N(5)-Tb(1)	2.431(6)	N(13)-O(1)	1.232(12)
N(6)-Tb(1)	2.424(6)	N(13)-O(2)	1.233(12)
N(7)-Tb(1)	2.439(6)	N(13)-O(3)	1.292(11)
N(8)-Tb(1)	2.410(6)	O(3)-Zn(1)	2.146(6)

N(9)-Tb(1)	2.513(6)	O(4)-Zn(1)	2.089(5)
N(10)-Tb(1)	2.524(6)	O(4)-Tb(1)	2.311(5)
N(11)-Zn(1)	2.046(7)	O(6)-Zn(1)	2.091(5)
N(12)-Zn(1)	2.109(7)	O(6)-Tb(1)	2.317(4)
N(11)-Zn(1)-O(4)	102.2(2)	N(6)-Tb(1)-N(7)	70.49(19)
N(11)-Zn(1)-O(6)	107.7(2)	N(5)-Tb(1)-N(7)	108.95(19)
O(4)-Zn(1)-O(6)	77.96(19)	O(4)-Tb(1)-N(9)	71.95(19)
N(11)-Zn(1)-N(12)	99.1(3)	O(6)-Tb(1)-N(9)	107.11(18)
O(4)-Zn(1)-N(12)	158.0(3)	N(8)-Tb(1)-N(9)	138.3(2)
O(6)-Zn(1)-N(12)	90.4(2)	N(6)-Tb(1)-N(9)	83.07(19)
N(11)-Zn(1)-O(3)	92.1(3)	N(5)-Tb(1)-N(9)	79.03(19)
O(4)-Zn(1)-O(3)	90.5(2)	N(7)-Tb(1)-N(9)	147.2(2)
O(6)-Zn(1)-O(3)	158.7(2)	O(4)-Tb(1)-N(10)	106.16(18)
N(12)-Zn(1)-O(3)	94.3(3)	O(6)-Tb(1)-N(10)	71.45(18)
O(4)-Tb(1)-N(8)	145.63(19)	N(6)-Tb(1)-N(10)	138.9(2)
O(6)-Tb(1)-N(8)	83.26(18)	N(5)-Tb(1)-N(10)	78.76(19)
O(4)-Tb(1)-N(6)	83.97(18)	N(7)-Tb(1)-N(10)	148.02(19)
N(8)-Tb(1)-N(6)	111.17(19)	O(4)-Tb(1)-N(7)	86.00(19)
O(4)-Tb(1)-N(5)	143.81(18)	O(6)-Tb(1)-N(7)	86.28(18)
O(6)-Tb(1)-N(5)	141.99(18)	N(8)-Tb(1)-N(7)	71.6(2)
N(8)-Tb(1)-N(5)	69.92(19)	N(6)-Tb(1)-N(5)	71.3(2)

The symmetry codes:
(a) x, y, -z-1/2, for **2**
(a) x, y, -z-1/2; (b) x-1, y, z; (c) x+1,y, z; (d) x+1, y, -z-1/2, for **3**
(a) x, y, -z-1/2; (b) x-1, y, z; (c) x+1, y, z; (d) x+1, y, -z-1/2, for **4**
(a) x, y, -z-1/2; (b) x-1, y, z; (c) x+1 ,y ,z; (d) x+1, y,-z-1/2, for **5**.

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Table S2. Analytical and mass spectroscopic data for the series of sandwich-type complexes **1-6** and **1-5** with Zn (II).[a]

Compound	M^+ (*m/z*)[d]	Analysis (%)		
		C	H	N
$C_{60}H_{50}LiN_{10}O_7Tb$ (**1**)[b]	1052.68 (1052.78)	59.87 (60.61)	4.13 (4.24)	12.04 (11.78)
$C_{55}H_{38}N_{10}NaO_5Tb$ (**2**)	1068.00 (1068.83)	60.11 (60.00)	3.56 (3.48)	12.52 (12.72)
$C_{55}H_{38}N_{10}KO_5Tb$ (**3**)	1083.39 (1084.94)	59.11 (59.14)	3.46 (3.43)	12.47 (12.54)
$C_{55}H_{38}N_{10}RbO_5Tb$ (**4**)	1131.56 (1131.31)	56.42 (56.78)	3.58 (3.29)	12.23 (12.04)
$C_{55}H_{38}N_{10}CsO_5Tb$ (**5**)	1178.05 (1178.74)	54.23 (54.56)	3.57 (3.16)	11.02 (11.57)
$C_{70}H_{60}N_{13}O_{10}TbZn$ (**6**)[c]	1110.33 (1111.22)	57.04 (57.28)	3.90 (4.12)	12.20 (12.41)
(**1**)+Zn(II)	1112.02 (1111.22)			
(**2**)+Zn(II)	1111.50 (1111.22)			
(**3**)+Zn(II)	1110.66 (1111.22)			
(**4**)+Zn(II)	1110.59 (1111.22)			
(**5**)+Zn(II)	1109.91 (1111.22)			

[a] Calculated values given in parentheses. [b] Contain 1.0 equiv of solvent tetrahydrofuran. [c] Contain 2.0 equiv of solvated CH_3OH, and 1.0 equiv of solvated tetrahydrofuran. [d] Experimental and calculated mass spectroscopic data for the these seven double-decker compounds **1-6** and complexes **1-5** with Zn (II) without one coordinated any coordinated solvent molecule, respectively.