Construction and characterization of rare earth complexes for efficient emission tuning by tetraethyl ethylenebisphosphonate and tridentate chelating nitrogen ligands

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Table S1 Experimental reagents, specifications and manufacturers

Reagents	Specifications	Manufacturers
$Ln(NO_3)_3 \cdot 6H_2O$ (Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy)	99.99%	Changcheng Chemical Technology Development Co., Ltd
Tetraethyl diphosphate ($C_{10}H_{24}O_6P_2$)	98.0%	Tokyo Kasei Industries, Ltd
Tripyridinetriazine ($C_{18}H_{12}N_6$)	98%	Changcheng Chemical Technology Development Co., Ltd
Acetonitrile (CH_3CN)	99%	Tianjin Zhiyuan Chemical Reagent Co., Ltd
Ethanol (C_2H_5OH)	99.7%	Tianjin Zhiyuan Chemical Reagent Co., Ltd

Methanol (CH_3OH)	99.7%	Tianjin Zhiyuan Chemical Reagent Co., Ltd

Table S2 Selected bond length (Å) and angles (°) for **1-10**

Complex 1	□	□	□	□	□
La(1)-O(10)	2.449(2)	La(1)-O(4)	2.626(3)	La(1)-O(5)	2.633(3)
La(1)-O(1)	2.580(3)	La(1)-N(2)	2.710(3)	La(1)-N(1)	2.656(3)
La(1)-O(2)	2.643(3)	La(1)-O(8)	2.618(3)	La(1)-N(3)	2.667(3)
La(1)-O(7)	2.637(3)	□	□	□	□
O(10)-La(1)-N(2)	137.98(9)	N(1)-La(1)-N(2)	61.14(9)	O(4)-La(1)-O(5)	47.85(10)
O(10)-La(1)-N(1)	81.89(9)	N(1)-La(1)-N(3)	120.96(9)	O(7)-La(1)-O(8)	48.31(9)
O(10)-La(1)-N(3)	142.29(9)	N(2)-La(1)-N(3)	60.81(8)	O(2)-La(1)-O(1)	48.63(9)
□	□	□	□	□	□
Complex 2	□	□	□	□	□
Ce(1)-O(10)	2.426(2)	Ce(1)-O(4)	2.598(3)	Ce(1)-O(5)	2.616(3)
Ce(1)-O(1)	2.551(3)	Ce(1)-N(2)	2.683(3)	Ce(1)-N(1)	2.643(3)
Ce(1)-O(2)	2.624(3)	Ce(1)-O(8)	2.594(3)	Ce(1)-N(3)	2.637(3)
Ce(1)-O(7)	2.612(3)	□	□	□	□
O(10)-Ce(1)-N(2)	138.10(8)	N(1)-Ce(1)-N(2)	61.41(8)	O(4)-Ce(1)-O(5)	48.34(9)
O(10)-Ce(1)-N(1)	141.98(9)	N(1)-Ce(1)-N(3)	122.06(9)	O(7)-Ce(1)-O(8)	48.89(9)
O(10)-Ce(1)-N(3)	81.49(9)	N(2)-Ce(1)-N(3)	61.65(8)	O(2)-Ce(1)-O(1)	48.92(9)
□	□	□	□	□	□
Complex 3	□	□	□	□	□
Pr(01)-O(10)	2.4076(19)	Pr(01)-O(4)	2.589(2)	Pr(01)-O(5)	2.580(2)
Pr(01)-O(1)	2.600(2)	Pr(01)-N(2)	2.647(2)	Pr(01)-N(1)	2.621(2)
Pr(01)-O(2)	2.566(2)	Pr(01)-O(8)	2.606(2)	Pr(01)-N(3)	2.613(2)
Pr(01)-O(7)	2.525(2)	□	□	□	□
O(10)-Pr(01)-N(2)	138.06(8)	N(1)-Pr(01)-N(2)	61.90(8)	O(4)-Pr(01)-O(5)	49.36(8)
O(10)-Pr(01)-N(1)	141.10(8)	N(1)-Pr(01)-N(3)	122.95(8)	O(7)-Pr(01)-O(8)	49.70(8)
O(10)-Pr(01)-N(3)	80.89(8)	N(2)-Pr(01)-N(3)	62.23(7)	O(2)-Pr(01)-O(1)	49.33(7)
□	□	□	□	□	□
Complex 4	□	□	□	□	□
Nd(01)-O(10)	2.3950(17)	Nd(01)-O(4)	2.5105(18)	Nd(01)-O(5)	2.5934(18)

Nd(01)-O(1)	2.5659(19)	Nd(01)-N(2)	2.6262(19)	Nd(01)-N(1)	2.599(2)
Nd(01)-O(2)	2.5816(18)	Nd(01)-O(8)	2.5478(19)	Nd(01)-N(3)	2.605(2)
Nd(01)-O(7)	2.5901(18)	□	□	□	□
O(10)-Nd(01)-N(2)	138.11(6)	N(1)-Nd(01)-N(2)	62.72(6)	O(4)-Nd(01)-O(5)	49.93(6)
O(10)-Nd(01)-N(1)	80.62(6)	N(1)-Nd(01)-N(3)	123.68(6)	O(7)-Nd(01)-O(8)	49.71(6)
O(10)-Nd(01)-N(3)	140.83(6)	N(2)-Nd(01)-N(3)	62.11(6)	O(2)-Nd(01)-O(1)	49.54(6)
□	□	□	□	□	□
Complex 5	□	□	□	□	□
Sm(1)-O(10)	2.362(3)	Sm(1)-O(4)	2.584(4)	Sm(1)-O(5)	2.539(4)
Sm(1)-O(1)	2.492(4)	Sm(1)-N(2)	2.604(4)	Sm(1)-N(1)	2.587(4)
Sm(1)-O(2)	2.577(4)	Sm(1)-O(8)	2.527(4)	Sm(1)-N(3)	2.588(4)
Sm(1)-O(7)	2.558(4)	□	□	□	□
O(10)-Sm(1)-N(2)	138.48(12)	N(1)-Sm(1)-N(2)	62.72(12)	O(4)-Sm(1)-O(5)	49.33(13)
O(10)-Sm(1)-N(1)	140.55(12)	N(1)-Sm(1)-N(3)	124.82(12)	O(7)-Sm(1)-O(8)	49.83(12)
O(10)-Sm(1)-N(3)	80.64(12)	N(2)-Sm(1)-N(3)	63.14(12)	O(2)-Sm(1)-O(1)	50.02(13)
□	□	□	□	□	□
Complex 6	□	□	□	□	□
Eu(1)-O(10)	2.349(2)	Eu(1)-O(4)	2.521(2)	Eu(1)-O(5)	2.583(3)
Eu(1)-O(1)	2.476(3)	Eu(1)-N(2)	2.589(2)	Eu(1)-N(1)	2.572(3)
Eu(1)-O(2)	2.573(3)	Eu(1)-O(8)	2.509(3)	Eu(1)-N(3)	2.571(3)
Eu(1)-O(7)	2.557(3)	□	□	□	□
O(10)-Eu(1)-N(2)	138.50(8)	N(1)-Eu(1)-N(2)	62.86(8)	O(4)-Eu(1)-O(5)	49.81(9)
O(10)-Eu(1)-N(1)	140.32(8)	N(1)-Eu(1)-N(3)	125.26(8)	O(7)-Eu(1)-O(8)	50.24(8)
O(10)-Eu(1)-N(3)	80.48(8)	N(2)-Eu(1)-N(3)	63.44(8)	O(2)-Eu(1)-O(1)	50.50(8)
□	□	□	□	□	□
Complex 7	□	□	□	□	□
Gd(1)-O(10)	2.314(4)	Gd(1)-O(4)	2.621(5)	Gd(1)-O(5)	2.468(5)
Gd(1)-O(1)	2.474(4)	Gd(1)-N(2)	2.546(5)	Gd(1)-N(1)	2.556(5)
Gd(1)-O(2)	2.592(5)	Gd(1)-O(8)	2.476(5)	Gd(1)-N(3)	2.537(6)
Gd(1)-O(7)	2.529(5)	□	□	□	□
O(10)-Gd(1)-N(2)	140.63(15)	N(1)-Gd(1)-N(2)	63.09(17)	O(4)-Gd(1)-O(5)	50.10(16)
O(10)-Gd(1)-N(1)	139.26(17)	N(1)-Gd(1)-N(3)	126.37(17)	O(7)-Gd(1)-O(8)	51.00(16)
O(10)-Gd(1)-N(3)	81.02(16)	N(2)-Gd(1)-N(3)	64.60(17)	O(2)-Gd(1)-O(1)	50.32(14)
□	□	□	□	□	□

Complex 8	□	□	□	□	□
Tb(1)-O(10)	2.315(2)	Tb(1)-O(4)	2.569(2)	Tb(1)-O(5)	2.444(3)
Tb(1)-O(1)	2.459(3)	Tb(1)-N(2)	2.536(3)	Tb(1)-N(1)	2.525(3)
Tb(1)-O(2)	2.596(3)	Tb(1)-O(8)	2.590(3)	Tb(1)-N(3)	2.542(3)
Tb(1)-O(7)	2.457(2)	□	□	□	□
O(10)-Tb(1)-N(2)	139.26(10)	N(1)-Tb(1)-N(2)	64.93(9)	O(4)-Tb(1)-O(5)	50.82(9)
O(10)-Tb(1)-N(1)	80.01(9)	N(1)-Tb(1)-N(3)	127.54(9)	O(7)-Tb(1)-O(8)	50.54(8)
O(10)-Tb(1)-N(3)	138.91(9)	N(2)-Tb(1)-N(3)	63.73(9)	O(2)-Tb(1)-O(1)	50.28(8)
□	□	□	□	□	□
Complex 9	□	□	□	□	□
Dy(1)-O(10)	2.290(2)	Dy(1)-O(4)	2.455(2)	Dy(1)-O(5)	2.513(2)
Dy(1)-O(1)	2.446(2)	Dy(1)-N(2)	2.518(3)	Dy(1)-N(1)	2.518(3)
Dy(1)-O(2)	2.582(2)	Dy(1)-O(8)	2.428(2)	Dy(1)-N(3)	2.551(3)
Dy(1)-O(7)	2.624(3)	□	□	□	□
O(10)-Dy(1)-N(2)	140.67(8)	N(1)-Dy(1)-N(2)	65.17(8)	O(4)-Dy(1)-O(5)	51.28(8)
O(10)-Dy(1)-N(1)	80.65(8)	N(1)-Dy(1)-N(3)	127.53(8)	O(7)-Dy(1)-O(8)	50.32(8)
O(10)-Dy(1)-N(3)	138.32(9)	N(2)-Dy(1)-N(3)	63.76(9)	O(2)-Dy(1)-O(1)	50.52(8)
□	□	□	□	□	□
Complex 10	□	□	□	□	□
Eu(1)-O(1)	2.371(7)	Eu(1)-O(4)	2.492(8)	Eu(1)-O(5)	2.635(8)
Eu(1)-O(7)	2.588(8)	Eu(1)-O(8)	2.481(9)	Eu(1)-O(10)	2.483(8)
Eu(1)-O(11)	2.572(8)	Eu(1)-N(1)	2.586(9)	Eu(1)-N(4)	2.610(9)
Eu(1)-N(5)	2.631(9)	□	□	□	□
O(1)-Eu(1)-N(4)	81.2(3)	N(1)-Eu(1)-N(4)	62.7(3)	O(4)-Eu(1)-N(5)	84.4(3)
O(1)-Eu(1)-N(1)	137.8(3)	N(1)-Eu(1)-N(5)	62.6(3)	O(7)-Eu(1)-O(8)	50.1(3)
O(1)-Eu(1)-N(5)	142.5(3)	N(4)-Eu(1)-N(5)	125.0(3)	O(10)-Eu(1)-O(11)	50.9(3)

Table S3. Weak interactions in complex **1**

Intermolecular hydrogen bonds in complex **1**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(4)-H(4)···O(9)	0.93	2.49	3.129(6)	126
C(9)-H(9)···O(5)	0.93	2.48	3.368(5)	160

C(13)-H(13)···O(7)	0.93	2.50	3.100(5)	122
C(14)-H(14)···O(9)	0.93	2.47	3.262(6)	143

Intramolecular hydrogen bonds in complex **1**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(1)-H(1)···O(10)	0.93	2.58	3.257(5)	130
C(16)-H(16A)···O(2)	0.97	2.54	3.475(5)	162
C(20)-H(20A)···O(3)	0.96	2.57	3.528(7)	177

Intermolecular π···π interaction in the stacking structure of complex **1**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(2)···Cg(3)	3.948(2)
Cg(3)···Cg(2)	3.948(2)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Cg(3) = N(3)-C(11)-C(12)-C(13)-C(14)-C(15)

Table S4. Weak interactions in complex **2**

Intermolecular hydrogen bonds in complex **2**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(2)-H(2)···O(9)	0.93	2.47	3.270(5)	145
C(3)-H(3)···O(7)	0.93	2.50	3.098(4)	123
C(7)-H(7)···O(5)	0.93	2.49	3.374(5)	159
C(12)-H(12)···O(9)	0.93	2.50	3.135(5)	125

Intramolecular hydrogen bonds in complex **2**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(15)-H(15)···O(10)	0.93	2.54	3.218(5)	130
C(16)-H(16B)···O(2)	0.97	2.54	3.471(4)	160
C(20)-H(20B)···O(3)	0.96	2.56	3.520(7)	177

Intermolecular π···π interaction in the stacking structure of complex **2**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(1)···Cg(2)	3.949(2)
Cg(2)···Cg(1)	3.949(2)

Cg(1) = N(1)-C(1)-C(2)-C(3)-C(4)-C(5)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Table S5. Weak interactions in complex **3**

Intermolecular hydrogen bonds in complex **3**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(2)-H(2)···O(3)	0.93	2.43	3.222(4)	143
C(3)-H(3)···O(1)	0.93	2.50	3.094(4)	122
C(7)-H(7)···O(4)	0.93	2.44	3.329(4)	159
C(13)-H(13)···O(6)	0.93	2.57	3.355(4)	142

Intramolecular hydrogen bonds in complex **3**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(15)-H(15)···O(10)	0.93	2.51	3.179(4)	129
C(16)-H(16B)···O(8)	0.97	2.55	3.475(4)	159
C(18)-H(18A)···O(9)	0.96	2.56	3.503(5)	169

Intermolecular π···π interaction in the stacking structure of complex **3**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(1)···Cg(2)	3.8694(18)
Cg(2)···Cg(1)	3.8694(18)

Cg(1) = N(1)-C(1)-C(2)-C(3)-C(4)-C(5)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Table S6. Weak interactions in complex **4**

Intermolecular hydrogen bonds in complex **4**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(3)-H(3)···O(3)	0.93	2.57	3.362(4)	143
C(9)-H(9)···O(2)	0.93	2.44	3.323(3)	159
C(12)-H(12)···O(2)	0.93	2.60	3.465(3)	156
C(13)-H(13)···O(7)	0.93	2.50	3.092(3)	122
C(14)-H(14)···O(9)	0.93	2.43	3.235(3)	145

Intramolecular hydrogen bonds in complex **4**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(1)-H(1)···O(10)	0.93	2.49	3.161(3)	129
C(16)-H(16B)···O(5)	0.97	2.56	3.475(3)	158
C(18)-H(18A)···O(6)	0.96	2.56	3.507(4)	171

Intermolecular π···π interaction in the stacking structure of complex **4**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(2)···Cg(3)	3.8715(14)
Cg(3)···Cg(2)	3.8716(14)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Cg(3) = N(3)-C(11)-C(12)-C(13)-C(14)-C(15)

Table S7. Weak interactions in complex **5**

Intermolecular hydrogen bonds in complex **5**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(2)-H(2)···O(9)	0.93	2.46	3.293(8)	150
C(3)-H(3)···O(7)	0.93	2.54	3.119(6)	120
C(7)-H(7)···O(4)	0.93	2.47	3.348(6)	158
C(12)-H(12)···O(9)	0.93	2.51	3.135(7)	124

Intramolecular hydrogen bonds in complex **5**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(15)-H(15)···O(10)	0.93	2.51	3.160(6)	127
C(16)-H(16B)···O(2)	0.97	2.56	3.465(6)	156
C(20)-H(20B)···O(3)	0.96	2.60	3.549(9)	171

Intermolecular π···π interaction in the stacking structure of complex **5**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(1)···Cg(2)	3.957(3)
Cg(2)···Cg(1)	3.956(3)

Cg(1) = N(1)-C(1)-C(2)-C(3)-C(4)-C(5)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Table S8. Weak interactions in complex **6**

Intermolecular hydrogen bonds in complex **6**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(2)-H(2)···O(9)	0.93	2.45	3.289(5)	151
C(3)-H(3)···O(7)	0.93	2.54	3.118(4)	121
C(7)-H(7)···O(5)	0.93	2.47	3.351(4)	158
C(12)-H(12)···O(9)	0.93	2.50	3.127(5)	125

Intramolecular hydrogen bonds in complex **6**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(15)-H(15)···O(10)	0.93	2.50	3.139(4)	126
C(16)-H(16B)···O(2)	0.97	2.55	3.451(4)	155
C(18)-H(18B)···O(3)	0.96	2.59	3.546(6)	174

Intermolecular π···π interaction in the stacking structure of complex **6**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(1)···Cg(2)	3.962(2)
Cg(2)···Cg(1)	3.962(2)

Cg(1) = N(1)-C(1)-C(2)-C(3)-C(4)-C(5)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Table S9. Weak interactions in complex **7**

Intermolecular hydrogen bonds in complex **7**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(3)-H(3)···O(7)	0.93	2.53	3.161(9)	125
C(4)-H(4)···O(2)	0.93	2.54	3.376(8)	150
C(7)-H(7)···O(2)	0.93	2.42	3.323(9)	162
C(12)-H(12)···O(5)	0.93	2.47	3.370(8)	162
C(17)-H(17B)···N(017)	0.97	2.61	3.456(17)	145
C(20)-H(20C)···O(3)	0.96	2.53	3.430(12)	156

Intramolecular hydrogen bonds in complex **7**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(1)-H(1)···O(1)	0.93	2.58	3.162(9)	121
C(15)-H(15)···O(10)	0.93	2.53	3.136(9)	124
C(16)-H(16A)···O(1)	0.97	2.61	3.456(17)	145

Intermolecular π···π interaction in the stacking structure of complex **7**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(2)···Cg(3)	3.760(4)
Cg(3)···Cg(2)	3.760(4)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Cg(3) = N(3)-C(11)-C(12)-C(13)-C(14)-C(15)

Table S10. Weak interactions in complex **8**

Intermolecular hydrogen bonds in complex **8**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(017)-H(01B)···O(7)	0.96	2.57	3.501(8)	164
C(12)-H(12)···O(2)	0.93	2.42	3.275(5)	153
C(13)-H(13)···O(8)	0.93	2.52	3.229(5)	133
C(14)-H(14)···O(9)	0.93	2.59	3.427(5)	149

Intramolecular hydrogen bonds in complex **8**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(1)-H(1)···O(10)	0.93	2.47	3.088(5)	124
C(16)-H(16B)···O(1)	0.97	2.41	3.264(4)	147
C(19)-H(19B)···O(1)	0.97	2.53	3.357(5)	144

Table S11. Weak interactions in complex **9**

Intermolecular hydrogen bonds in complex **9**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(016)-H(01C)···O(11)	0.96	2.59	3.486(8)	155
C(4)-H(4)···O(8)	0.93	2.50	3.391(4)	161
C(9)-H(9)···O(2)	0.93	2.42	3.314(4)	162
C(12)-H(12)···O(2)	0.93	2.52	3.365(4)	152
C(13)-H(13)···O(5)	0.93	2.56	3.169(4)	123
C(18)-H(18A)···O(3)	0.96	2.54	3.437(6)	156
C(19)-H(19A)···N(017)	0.97	2.62	3.460(8)	145

Intramolecular hydrogen bonds in complex **9**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(1)-H(1)···O(10)	0.93	2.51	3.107(5)	122
C(15)-H(15)···O(1)	0.93	2.57	3.140(4)	120
C(16)-H(16B)···O(1)	0.97	2.49	3.331(4)	145
C(19)-H(19B)···O(3)	0.97	2.60	3.467(5)	149

Intermolecular π···π interaction in the stacking structure of complex **9**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(1)···Cg(2)	3.7689(18)
Cg(2)···Cg(1)	3.7689(18)

Cg(1) = N(1)-C(1)-C(2)-C(3)-C(4)-C(5)

Cg(2) = N(2)-C(6)-C(7)-C(8)-C(9)-C(10)

Table S12. Weak interactions in complex **10**

Intermolecular hydrogen bonds in complex **10**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
C(11)-H(11)...O(5)	0.93	2.58	3.2460	129
C(12)-H(12)...O(11)	0.93	2.48	3.3345	153
C(13)-H(13)...O(12)	0.93	2.50	3.4066	164
C(18)-H(18)...O(10)	0.93	2.38	3.3098	173

Intramolecular hydrogen bonds in complex **10**

Donor-H···Acceptor	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)

C(1)-H(1B)...O(4)	0.97	2.52	3.3256	140
C(16)-H(16)...N(2)	0.93	2.45	2.7820	101
C(20)-H(20B)...O(4)	0.97	2.41	3.3206	157

Intermolecular π···π interaction in the stacking structure of complex **10**

Cg(I)···Cg(J)	Cg(I)-Cg(J) (Å)
Cg(2)···Cg(2)	3.8311
Cg(3)···Cg(3)	3.7046

Cg(2)= N(4)-C(5)-C(6)-C(7)-C(8)-C(9)

Cg(3)= N(5)-C(10)-C(11)-C(12)-C(13)-C(14)

Table S13. Key bond lengths and bond angles of reported similar complexes

Eu^{3+} complexes		
$[Eu(DMF)_2(C_{15}H_{11}N_3)(H_2O)_2(NO_3)]Pt(CN)_4$	Eu–N (TPY, average)	2.571 Å
	N1-Eu-N3	124.7°
	N2-Eu-N3	63.5°
$[EuL(Phen)Cl_3]_n$	Eu–O (L)	2.330 Å
$\{[Eu(tptz)(H_2O)_4Fe(CN)_6]\cdot 6H_2O\}_\infty$	Eu–N (TPTZ, average)	2.603 Å
	N4-Eu-N5	124.7°
	N1-Eu-N4	62.5°
$[EuL(Phen)Cl_3]_n$	Eu–O (L)	2.330 Å

Tb^{3+} complexes		
$[Tb(DMF)_2(C_{15}H_{11}N_3)(H_2O)_2(NO_3)]Pt(CN)_4$	Tb–N (TPY, average)	2.55 Å
	N1-Tb-N3	125.5°
	N2-Tb-N3	63.3°
$[TbL(Phen)Cl_3]_n$	Tb–O (L)	2.31 Å

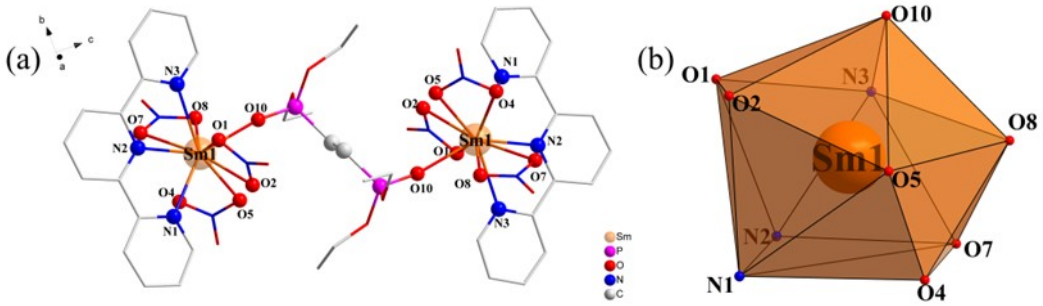


Fig. S1 (a) Diagram of the monomolecular structure of complex **5**; (b) coordination mode of Sm^{3+} in complex **5**.

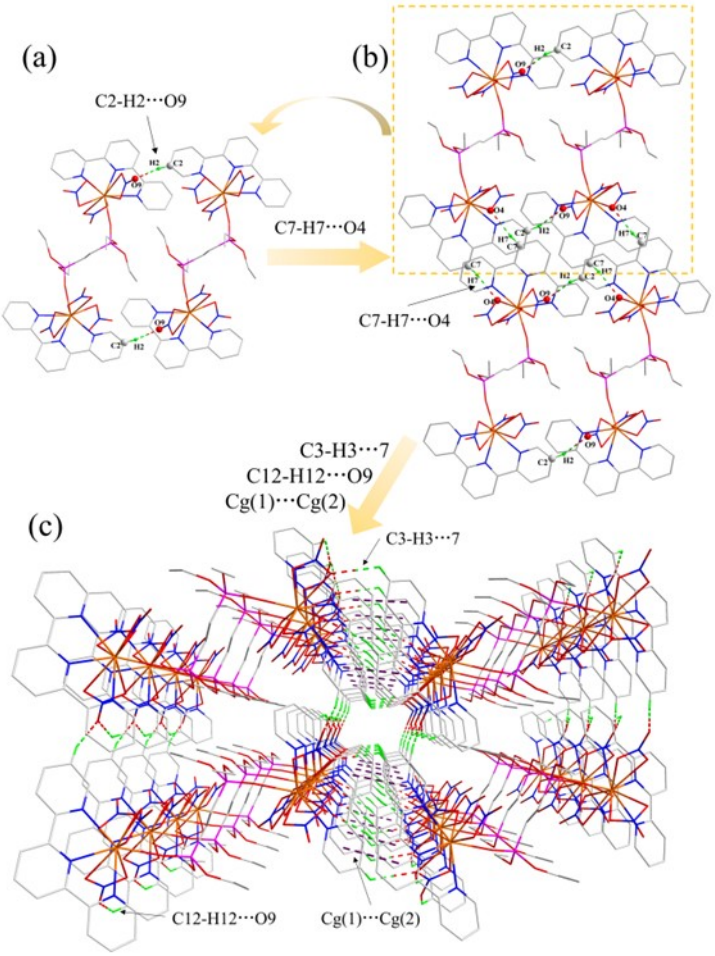
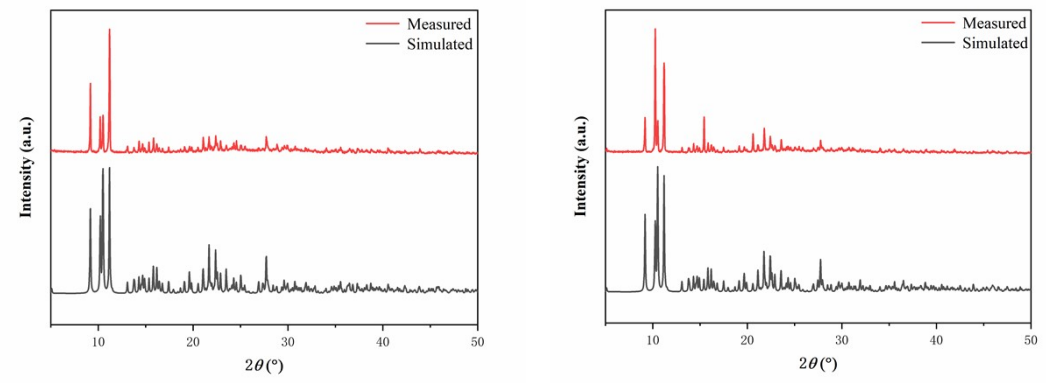
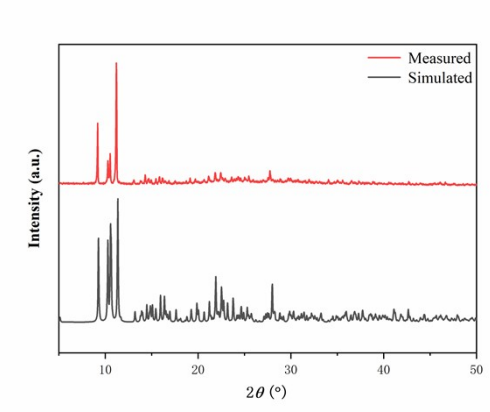


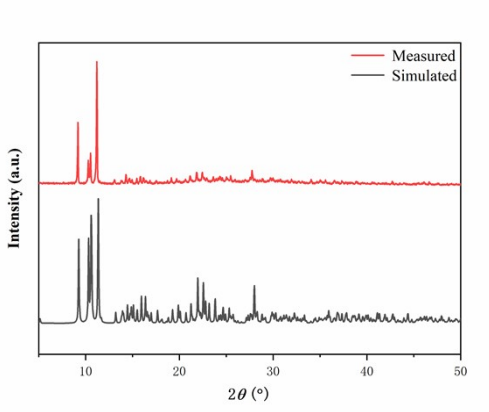
Fig. S2 (a) 1D infinite chain in complex **5**; (b) 2D planar structure in complex **5**; (c) 3D spatial structure in complex **5**.



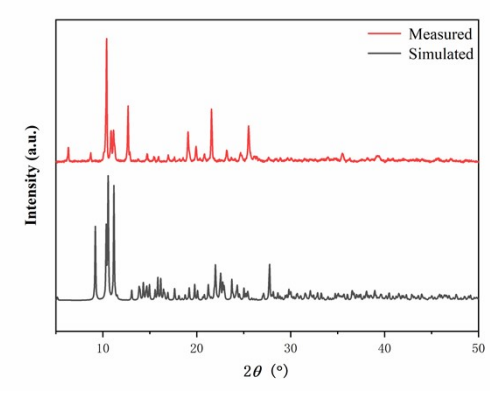
(a) (b)


Measured
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ (°)

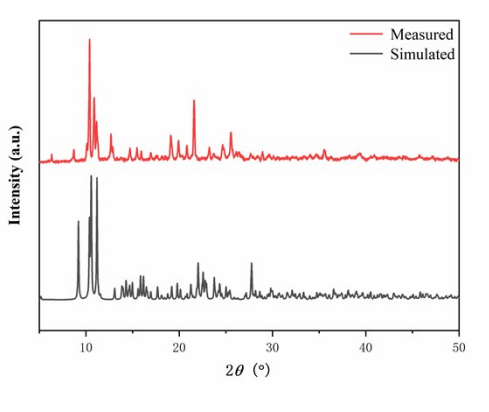
(c)


Measured
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ (°)

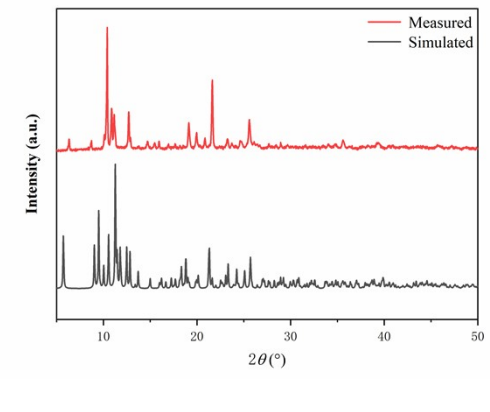
(d)


Measured
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ (°)

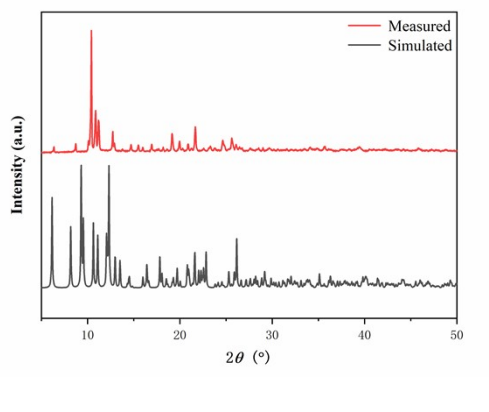
(e)


Measured
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ (°)

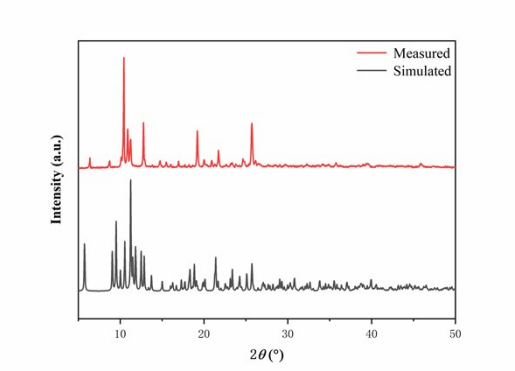
(f)


Measured
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ(°)

(g)


Measured
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ (°)

(h)



(i)

Fig. S3 PXRD plot of complexes **1-9** (a-i).

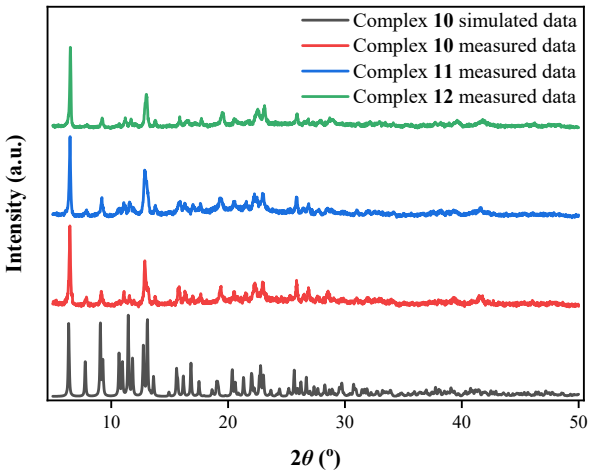
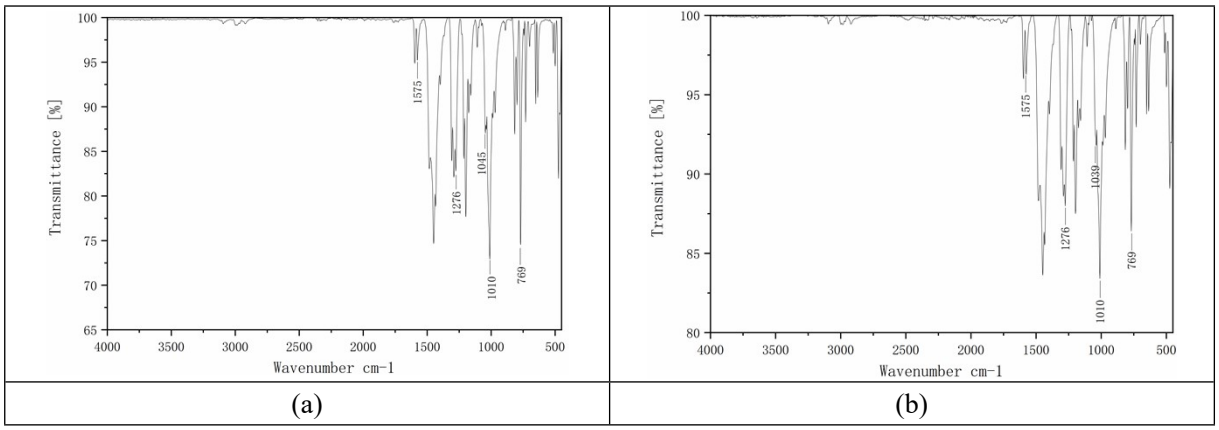
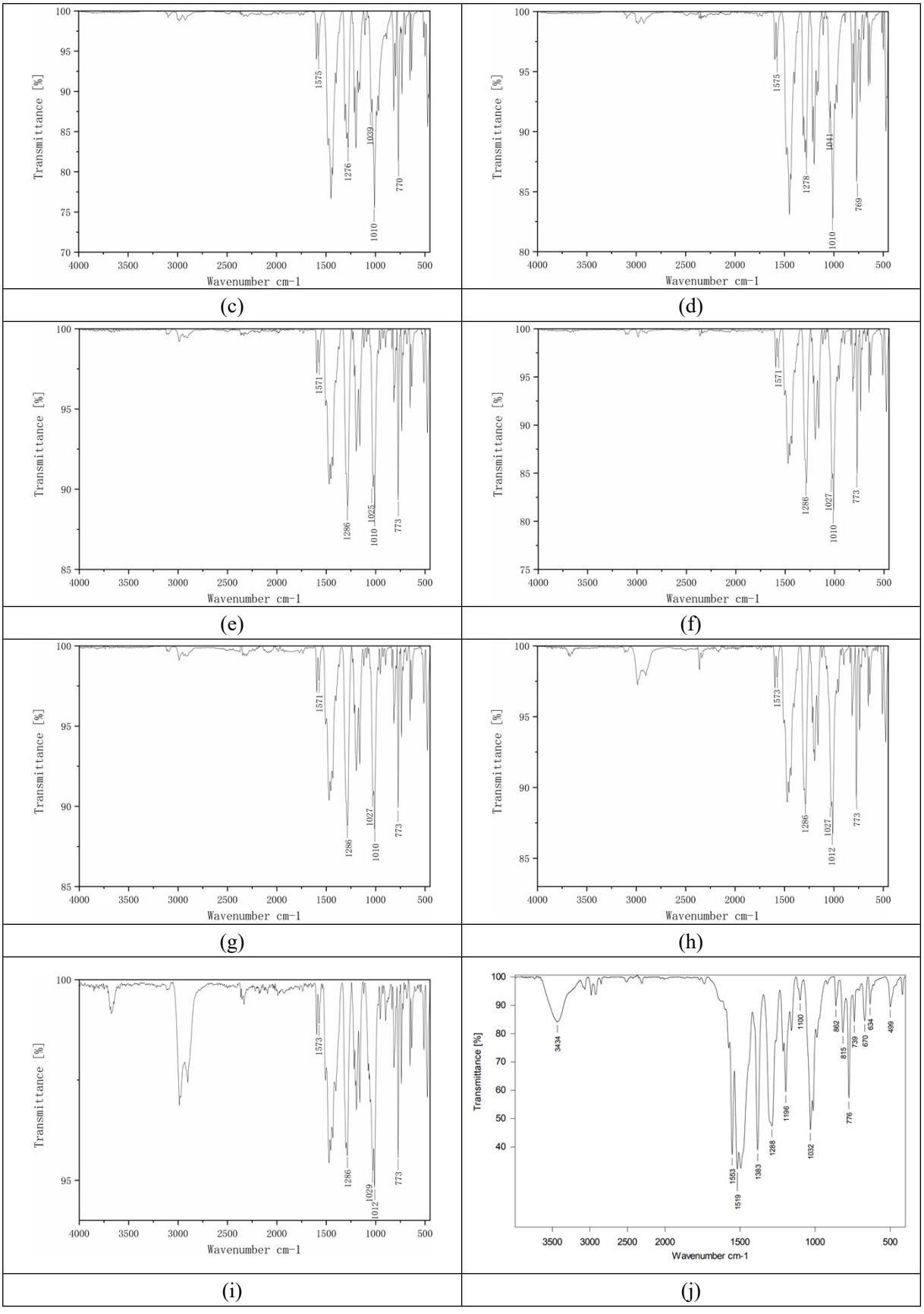


Fig. S4 PXRD plot of complexes **10-12**.



(a) (b)


Transmittance [%]
Wavenumber cm-1
1575
1276
1039
1010
770
(c)
1575
1278
1041
1010
769
(d)
1571
1286
1025
1010
773
(e)
1571
1286
1027
1010
773
(f)
1571
1286
1027
1010
773
(g)
1573
1286
1027
1012
773
(h)
1573
1286
1029
1012
773
(i)
3434
1553
1519
1383
1288
1196
1100
1032
862
815
776
739
670
634
499
(j)

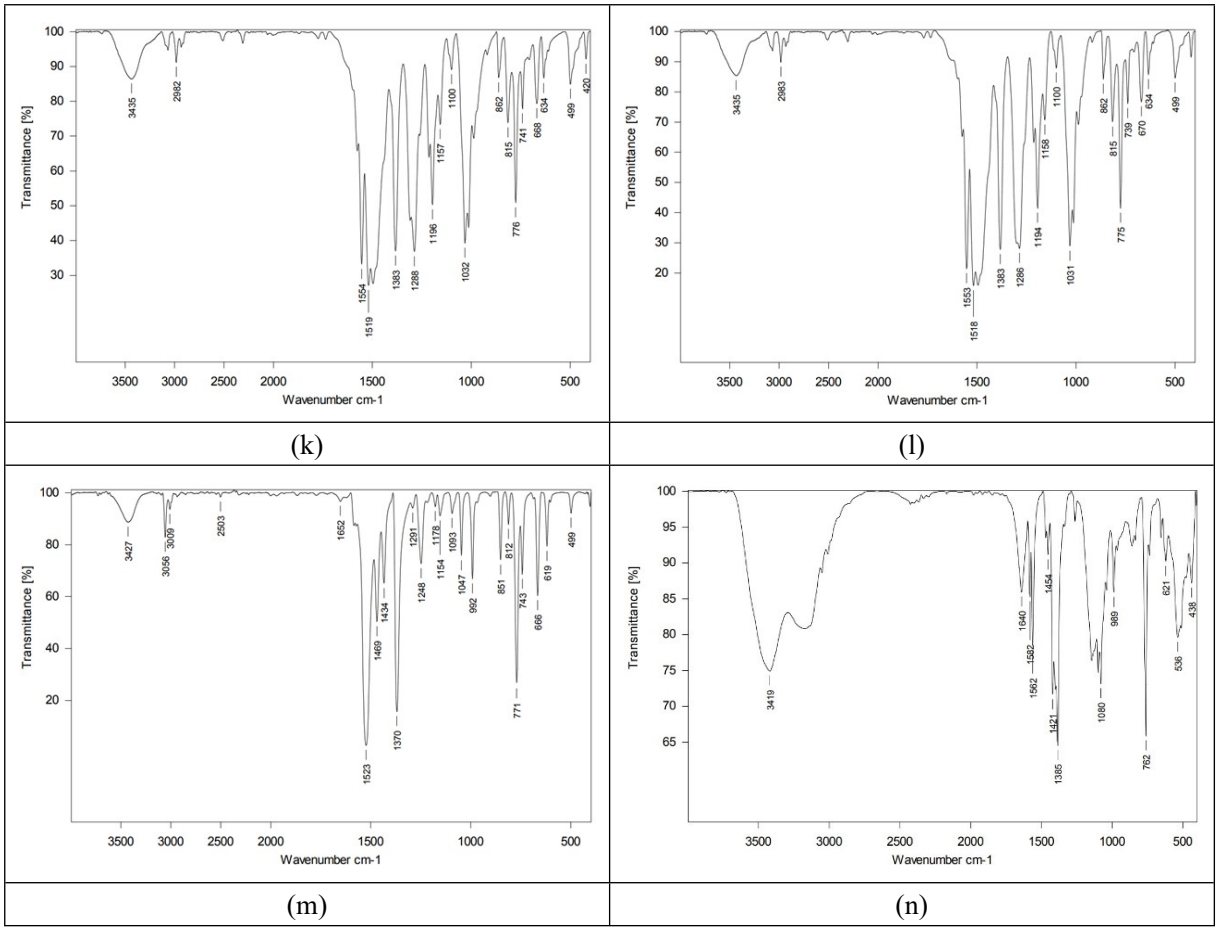


Fig. S5 Infrared spectrum of complex 1-12 (a-l), TPTZ (m) and TPY (n)

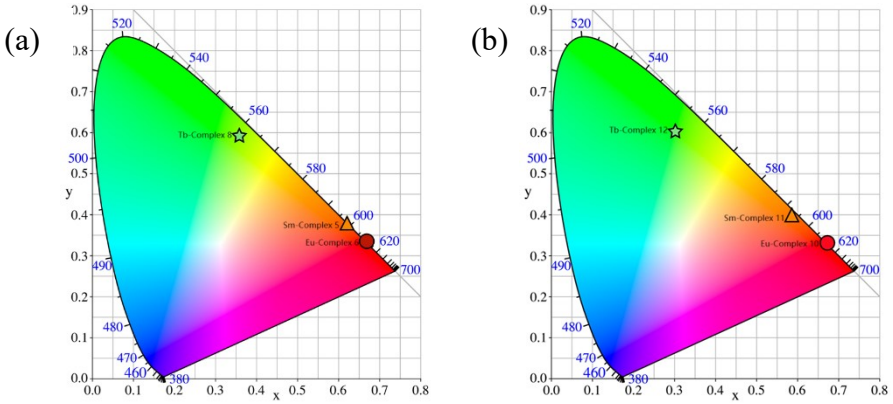


Fig. S6 Chromatic coordinates of (a) complexes **5**, **6**, **8** and (b) complexes **10**, **11**, **12**

THz spectroscopy properties

At room temperature, the terahertz spectra of L ligands, TPY ligands, and complexes 1-9 in the range of 0.4-2.4 THz were tested. All of the above compounds have characteristic formant peaks, which can arise from hydrogen bonding, dipole rotation, van der Waals

forces, low-frequency vibrations of the lattice, resulting in intense absorption and dispersion. The measured signal is obtained after a terahertz pulse is absorbed and scattered through the sample.

The terahertz spectra of L ligand, TPY ligand, and complex 1 are shown in Fig. SA. All three showed a downward trend, and there were many small absorption peaks in the terahertz spectra of L ligand and TPY ligand, which disappeared or moved after the formation of complex 1, which could be attributed to the generation of new structures and intermolecular interactions.

The terahertz spectra of complexes 7-9 and complexes 1-6 have almost identical peak shapes and trends, as shown in Fig. SB. The evaporation of the non-coordinated acetonitrile from complexes 7-9 could explain the identical structures of all nine test samples, leading to similar terahertz spectra. In addition, the peak intensities and peak shapes of the terahertz spectra of complexes 1-9 are slightly different, reflecting different intermolecular forces. Due to the many hydrogen bonds in the complex, it is not easy to identify peaks in the terahertz region. The relationship between terahertz spectroscopy and the structure and properties of complexes needs to be further explored. The experimental results in this paper complement the terahertz spectral properties of rare earth complexes.

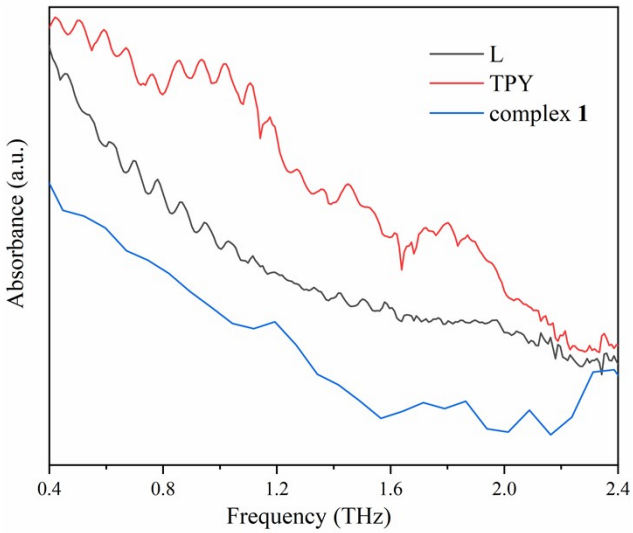
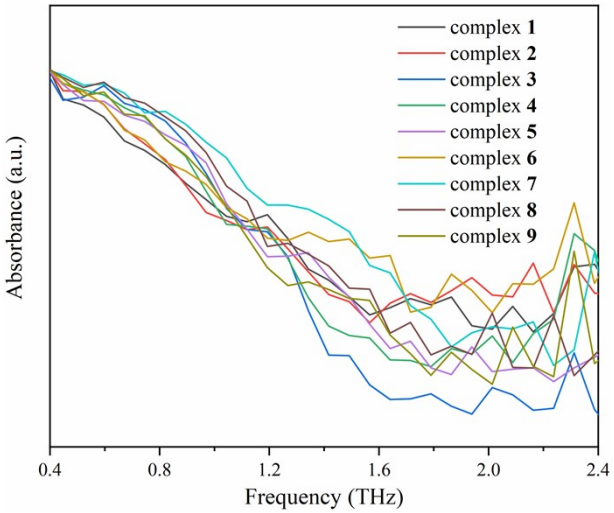


Fig. S7 Terahertz spectra of L ligand, TPY ligand, and complex **1**



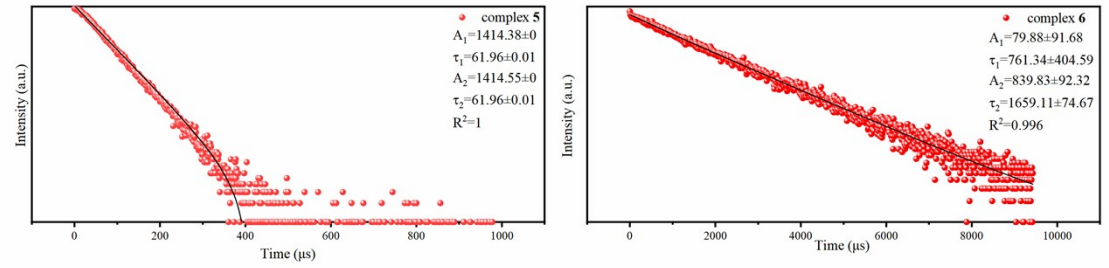


Fig. S8 Terahertz spectra of complexes **1-9**

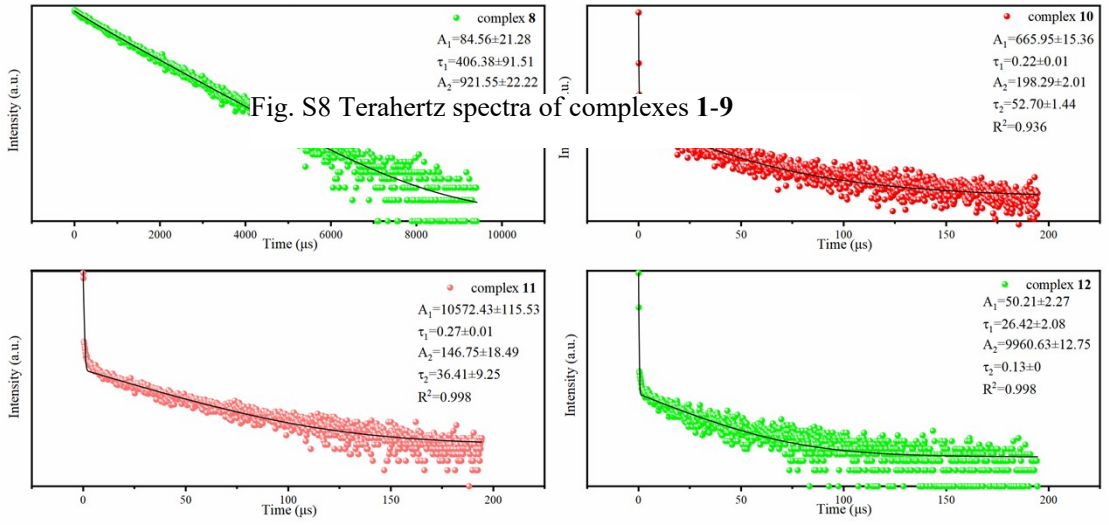


Fig. S9 Photoluminescent decay curves along with their corresponding fitting parameters

Calculation method of ϕ

The quantum yield (ϕ) is by definition, the photons emitted to the photons absorbed:

$$A = \frac{L_b - L_c}{L_b}$$

$$\phi = \frac{E_c - (1 - A) \cdot E_b}{L_a \cdot A} = \frac{E_c - E_a}{L_a - L_c}$$

where A is film absorbance, and L_b is the integrated excitation profile when the sample is diffusely illuminated by the integrating sphere's surface, and L_c is the integrated excitation profile when the sample is directly excited by the incident beam, and E_c is the integrated luminescence of the film caused by direct excitation, and E_b is the integrated luminescence of the film caused by indirect illumination from the sphere, and L_a is the integrated excitation profile from an empty integrating sphere (without the sample, only a blank), and E_a is the integrated luminescence from an empty integrating sphere (only a blank).