

Supporting Information

Syntheses, Structures, Near-Infrared and Visible Luminescence of Lanthanide-Organic Frameworks with Flexible Macrocyclic Polyamine Ligands

Xiandong Zhu ^{a, b}, Jian Lü ^{a, b}, Xiaoju Li ^{a, b}, Shuiying Gao ^{a, b}, Guoliang Li
^{a, b}, Fuxian Xiao ^{a, b}, Rong Cao* ^a

^aState Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fujian, Fuzhou, 350002, P. R. China; ^bGraduate School, Chinese Academy of Sciences, Beijing, 100039, P. R. China.

*Correspondence author. Fax: +86-591-83796710. E-mail: rcao@fjirsm.ac.cn.

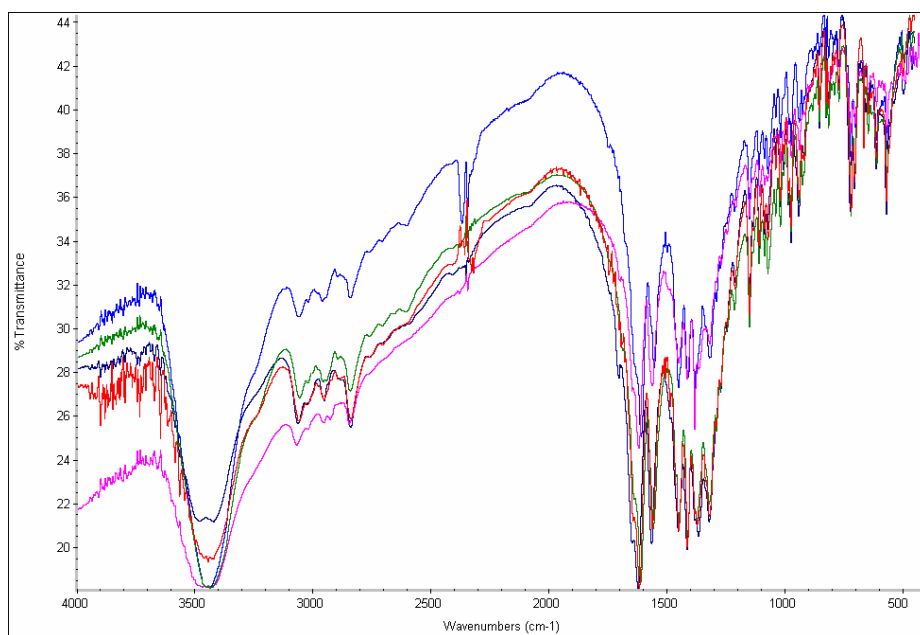


Figure S1. FT-IR spectra for complexes **1** (blue), **2** (dark blue), **3** (purple), **4** (green) and **5** (red).

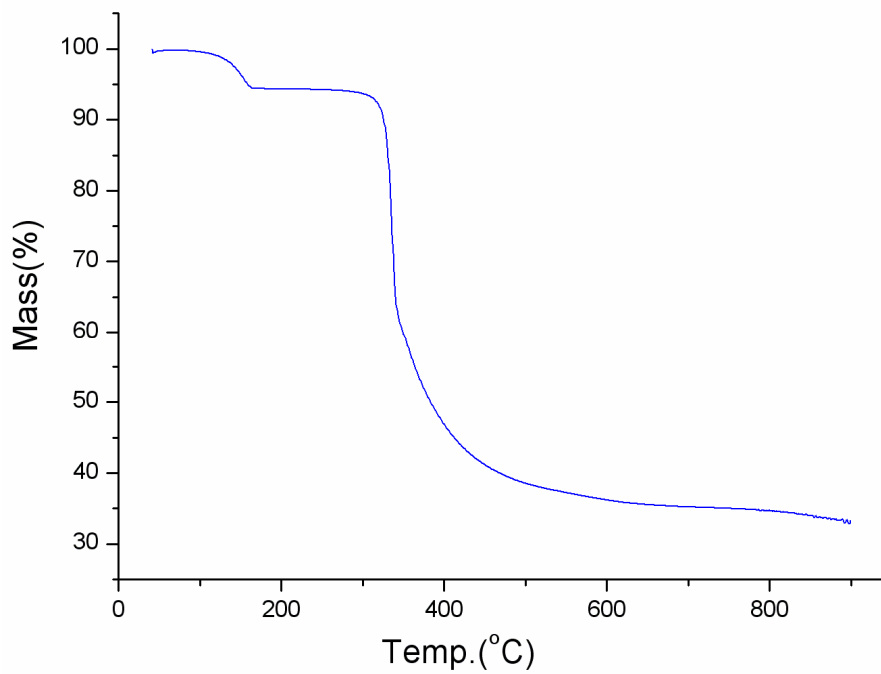


Figure S2. TGA curve for complex **1**.

Table S1. Selected Bond Lengths [Å] and Angles [°] for Complex **2^a**.

Eu(1)–O(1)	2.430(3)	Eu(1)–O(8)#1	2.334(3)
Eu(1)–O(6)#2	2.340(3)	Eu(1)–O(3)#3	2.397(3)
Eu(1)–O(4)#4	2.454(3)	Eu(1)–O(7)#5	2.478(3)
Eu(1)–O(2)#6	2.490(3)	Eu(1)–O(5)	2.513(3)
O(8)#1–Eu(1)–O(6)#2	145.83(11)	O(8)#1–Eu(1)–O(3)#3	139.02(11)
O(6)#2–Eu(1)–O(3)#3	74.46(10)	O(8)#1–Eu(1)–O(1)	72.75(10)
O(6)#2–Eu(1)–O(1)	140.62(10)	O(3)#3–Eu(1)–O(1)	69.82(10)
O(8)#1–Eu(1)–O(4)#4	78.10(10)	O(6)#2–Eu(1)–O(4)#4	74.99(11)
O(3)#3–Eu(1)–O(4)#4	122.84(10)	O(1)–Eu(1)–O(4)#4	139.68(10)
O(8)#1–Eu(1)–O(7)#5	114.68(10)	O(6)#2–Eu(1)–O(7)#5	77.58(11)
O(3)#3–Eu(1)–O(7)#5	71.35(10)	O(1)–Eu(1)–O(7)#5	75.80(10)
O(4)#4–Eu(1)–O(7)#5	143.10(11)	O(8)#1–Eu(1)–O(2)#6	73.58(10)
O(6)#2–Eu(1)–O(2)#6	78.42(10)	O(3)#3–Eu(1)–O(2)#6	142.88(10)
O(1)–Eu(1)–O(2)#6	123.07(9)	O(4)#4–Eu(1)–O(2)#6	72.26(10)
O(7)#5–Eu(1)–O(2)#6	78.46(10)	O(8)#1–Eu(1)–O(5)	72.80(10)
O(6)#2–Eu(1)–O(5)	116.44(11)	O(3)#3–Eu(1)–O(5)	81.48(10)
O(1)–Eu(1)–O(5)	74.27(10)	O(4)#4–Eu(1)–O(5)	70.85(10)
O(7)#5–Eu(1)–O(5)	144.96(10)	O(2)#6–Eu(1)–O(5)	134.03(10)

^a Symmetry transformations used to generate equivalent atoms: (#1) -x,-y+1,-z; (#2) -x,-y,-z; (#3) -x,-y,-z+1; (#4) x,y,z-1; (#5) x+1,y-1,z; (#6) -x+1,-y,-z.

Table S2. Selected Bond Lengths [Å] and Angles [°] for Complex **3^a**.

Tb(1)–O(1)	2.305(6)	Tb(1)–O(4)#1	2.310(6)
Tb(1)–O(6)#2	2.370(5)	Tb(1)–O(7)#2	2.415(5)
Tb(1)–O(5)	2.430(5)	Tb(1)–O(2)#3	2.442(6)
Tb(1)–O(8)#4	2.446(5)	Tb(1)–O(3)#5	2.463(6)
O(1)–Tb(1)–O(4)#1	145.5(2)	O(1)–Tb(1)–O(6)#2	138.7(2)
O(4)#1–Tb(1)–O(6)#2	74.7(2)	O(1)–Tb(1)–O(7)#2	73.42(19)
O(4)#1–Tb(1)–O(7)#2	140.16(19)	O(6)#2–Tb(1)–O(7)#2	70.21(18)
O(1)–Tb(1)–O(5)	77.9(2)	O(4)#1–Tb(1)–O(5)	74.5(2)
O(6)#2–Tb(1)–O(5)	121.66(18)	O(7)#2–Tb(1)–O(5)	141.2(2)
O(1)–Tb(1)–O(2)#3	115.5(2)	O(4)#1–Tb(1)–O(2)#3	76.9(2)
O(6)#2–Tb(1)–O(2)#3	73.23(19)	O(7)#2–Tb(1)–O(2)#3	75.5(2)
O(5)–Tb(1)–O(2)#3	141.8(2)	O(1)–Tb(1)–O(8)#4	74.3(2)
O(4)#1–Tb(1)–O(8)#4	78.1(2)	O(6)#2–Tb(1)–O(8)#4	143.1(2)
O(7)#2–Tb(1)–O(8)#4	121.84(18)	O(5)–Tb(1)–O(8)#4	72.89(19)

O(2)#3–Tb(1)–O(8)#4	76.77(19)	O(1)–Tb(1)–O(3)#5	72.5(2)
O(4)#1–Tb(1)–O(3)#5	116.3(2)	O(6)#2–Tb(1)–O(3)#5	80.11(19)
O(7)#2–Tb(1)–O(3)#5	75.61(19)	O(5)–Tb(1)–O(3)#5	71.2(2)
O(2)#3–Tb(1)–O(3)#5	145.81(19)	O(8)#4–Tb(1)–O(3)#5	135.06(19)

^a Symmetry transformations used to generate equivalent atoms: (#1) x+1,y+1,z; (#2) -x+1,-y+1,-z+1; (#3) -x,-y+1,-z+1; (#4) x-1,y,z; (#5) -x,-y,-z+1.

Table S3. Selected Bond Lengths [Å] and Angles [°] for Complex **4^a**.

Dy(1)–O(1)	2.422(3)	Dy(1)–O(4)#5	2.412(3)
Dy(1)–O(6)#1	2.285(3)	Dy(1)–O(7)#6	2.427(3)
Dy(1)–O(8)#2	2.285(3)	Dy(1)–O(5)	2.447(3)
Dy(1)–O(2)#4	2.404(3)	Dy(1)–O(3)#3	2.346(3)
O(6)#1–Dy(1)–O(8)#2	145.36(13)	O(4)#5–Dy(1)–O(1)	73.05(11)
O(6)#1–Dy(1)–O(3)#3	74.84(12)	O(6)#1–Dy(1)–O(7)#6	76.92(12)
O(8)#2–Dy(1)–O(3)#3	138.60(12)	O(8)#2–Dy(1)–O(7)#6	115.62(12)
O(6)#1–Dy(1)–O(2)#4	140.06(12)	O(3)#3–Dy(1)–O(7)#6	73.76(11)
O(8)#2–Dy(1)–O(2)#4	73.65(11)	O(2)#4–Dy(1)–O(7)#6	75.24(12)
O(3)#3–Dy(1)–O(2)#4	70.25(11)	O(4)#5–Dy(1)–O(7)#6	141.48(12)
O(6)#1–Dy(1)–O(4)#5	74.37(12)	O(1)–Dy(1)–O(7)#6	76.39(11)
O(8)#2–Dy(1)–O(4)#5	77.77(12)	O(6)#1–Dy(1)–O(5)	116.06(12)
O(3)#3–Dy(1)–O(4)#5	121.41(11)	O(8)#2–Dy(1)–O(5)	72.62(12)
O(2)#4–Dy(1)–O(4)#5	141.67(11)	O(3)#3–Dy(1)–O(5)	79.61(12)
O(6)#1–Dy(1)–O(1)	78.20(12)	O(2)#4–Dy(1)–O(5)	76.16(11)
O(8)#2–Dy(1)–O(1)	74.27(12)	O(4)#5–Dy(1)–O(5)	71.25(11)
O(3)#3–Dy(1)–O(1)	143.40(12)	O(1)–Dy(1)–O(5)	135.29(11)
O(2)#4–Dy(1)–O(1)	121.36(11)	O(7)#6–Dy(1)–O(5)	146.03(11)

^a Symmetry transformations used to generate equivalent atoms: (#1) -x+2,-y+1,-z; (#2) -x+3,-y+2,-z; (#3) x-1,y,z-1; (#4) -x+3,-y+1,-z; (#5) -x+3,-y+1,-z+1; (#6) x,y-1,z.

Table S4. Selected Bond Lengths [Å] and Angles [°] for Complex **5^a**.

Y(1)–O(1)	2.389(3)	Y(1)–O(4)#4	2.396(3)
Y(1)–O(5)#1	2.275(3)	Y(1)–O(6)	2.409(4)
Y(1)–O(8)#2	2.275(4)	Y(1)–O(2)#1	2.411(3)
Y(1)–O(3)#3	2.337(3)	Y(1)–O(7)#5	2.440(3)
O(5)#1–Y(1)–O(8)#2	145.33(13)	O(4)#4–Y(1)–O(6)	141.50(13)

O(5)#1–Y(1)–O(3)#3	138.51(13)	O(5)#1–Y(1)–O(2)#1	74.33(12)
O(8)#2–Y(1)–O(3)#3	74.92(13)	O(8)#2–Y(1)–O(2)#1	78.08(13)
O(5)#1–Y(1)–O(1)	73.75(12)	O(3)#3–Y(1)–O(2)#1	143.51(13)
O(8)#2–Y(1)–O(1)	139.89(13)	O(1)–Y(1)–O(2)#1	121.03(12)
O(3)#3–Y(1)–O(1)	70.35(12)	O(4)#4–Y(1)–O(2)#1	73.37(12)
O(5)#1–Y(1)–O(4)#4	77.76(13)	O(6)–Y(1)–O(2)#1	76.11(12)
O(8)#2–Y(1)–O(4)#4	74.50(13)	O(5)#1–Y(1)–O(7)#5	72.71(12)
O(3)#3–Y(1)–O(4)#4	121.05(12)	O(8)#2–Y(1)–O(7)#5	116.27(13)
O(1)–Y(1)–O(4)#4	141.85(12)	O(3)#3–Y(1)–O(7)#5	79.15(12)
O(5)#1–Y(1)–O(6)	115.64(13)	O(1)–Y(1)–O(7)#5	76.31(12)
O(8)#2–Y(1)–O(6)	76.72(13)	O(4)#4–Y(1)–O(7)#5	71.31(12)
O(3)#3–Y(1)–O(6)	74.15(12)	O(6)–Y(1)–O(7)#5	145.93(12)
O(1)–Y(1)–O(6)	75.04(12)	O(2)#1–Y(1)–O(7)#5	135.65(12)

^a Symmetry transformations used to generate equivalent atoms: (#1) -x,-y,-z+1; (#2) -x+1,-y+1,-z+1; (#3) -x+1,-y,-z+2; (#4) x,y,z-1; (#5) x,y-1,z.