Supporting Information

Construction of NIR luminescent polynuclear lanthanide-based nanoclusters with sensing properties towards metal ions

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Contents

1. General Procedures

Metal salts and solvents were purchased from Meryer and used directly without further purification. All reactions were performed under dry oxygen-free dinitrogen atmospheres using standard Schlenk techniques. Physical measurements: Powder XRD: D8ADVANCE; IR: Nicolet IS10 spectrometer. Melting points were obtained in sealed glass capillaries under dinitrogen and are uncorrected. Elemental analyses (C, H, N) were carried out on a EURO EA3000 elemental analysis. Field emission scanning electron microscopy (FESEM) images and EDX spectra were recorded on a Nova NanoSEM 200 scanning electron microscope.

2. ^{1}H NMR spectrum of H_2L^1 and H_2L^2

^{1}H NMR experiments were performed on a Bruker Avance III NMR spectrometer at 500.13MHz, equipped with a 5 mm room temperature probe (Bruker Instruments Inc., Germany), and reported as parts per million (ppm) from the internal standard TMS (solvent, $CDCl_3$). The experimental conditions are as follows: spectrometer frequency 500.13 MHz, spectral width (SW) 10 ppm, pulse 90°, acquisition time (AQ) 5.40 s, relaxation delay (RD) 2.00 s, and Fourier Transform (FT) size 32K data point. An exponential window function with a line-broadening factor of 1 Hz was applied to the FID before Fourier transformation.

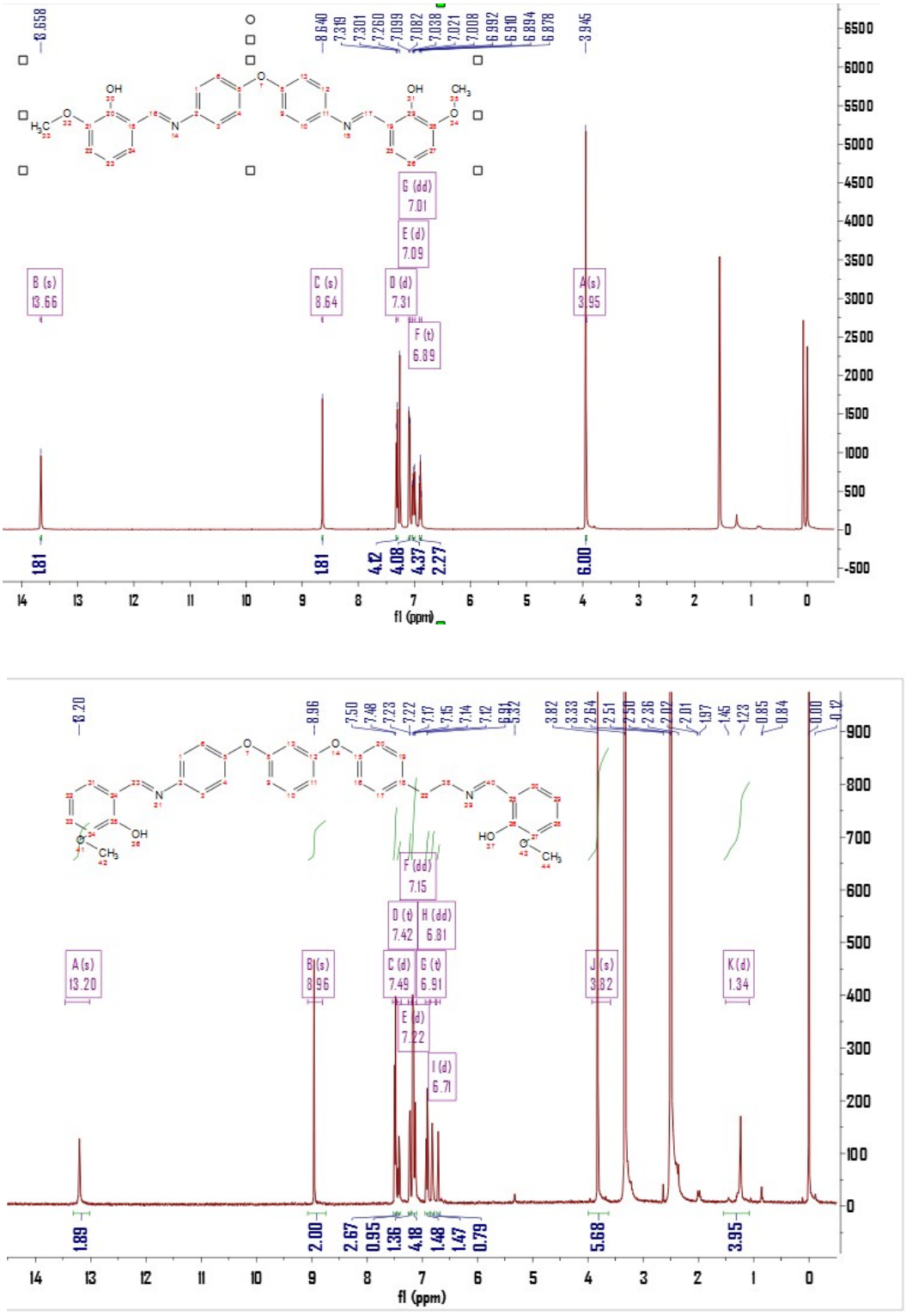
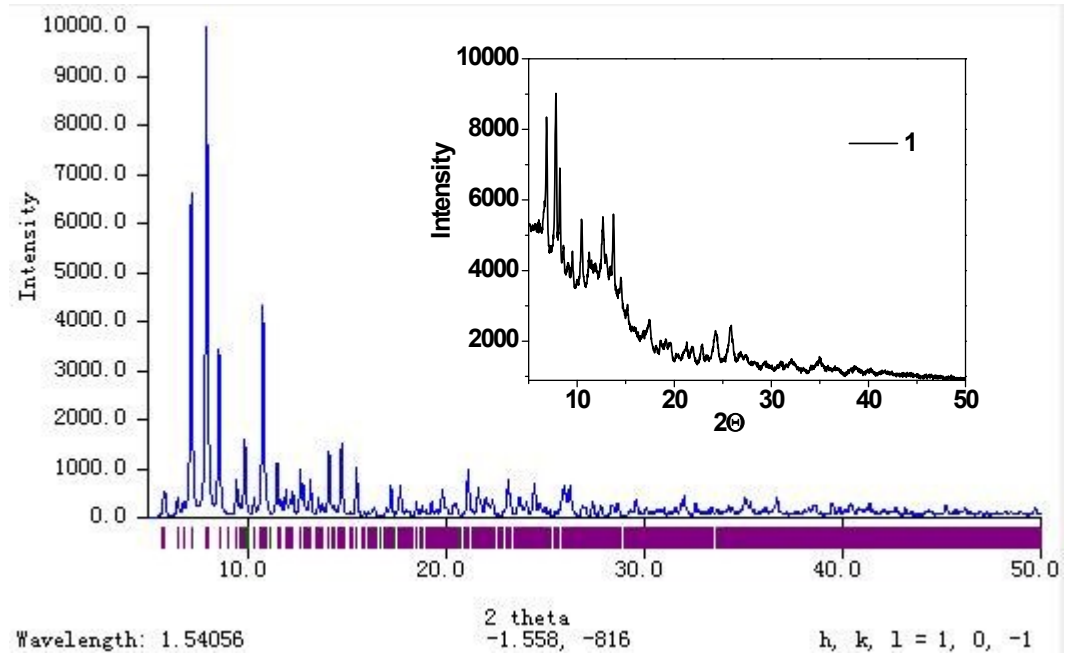


Figure S1. ^{1}HNMR spectra of H_2L^1 in $CDCl_3$ and H_2L^2in DMSO.

3. Powder XRD patterns of 1 and 3



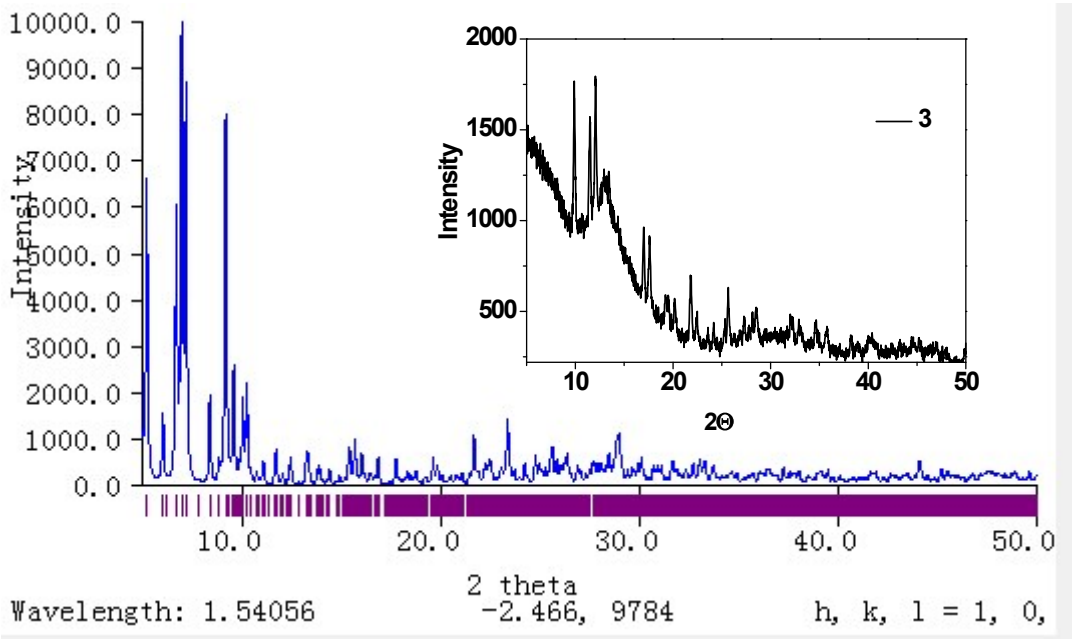


Figure S2. Powder XRD patterns of **1** and **3** (the insert pictures were obtained from experiments).

4. The IR spectra of $H_2L^{1,2}$ and 1-3

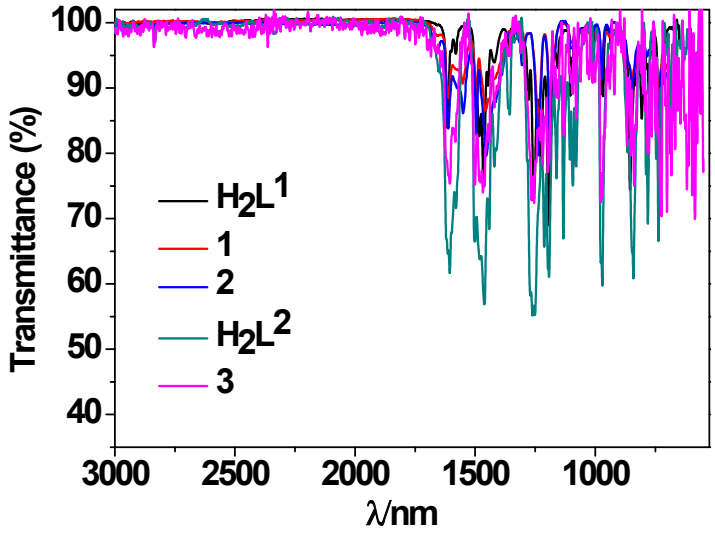


Figure S3. Infrared spectra of $H_2L^{1,2}$ and **1-3**.

5. SEM image and EDX spectrum of 2.

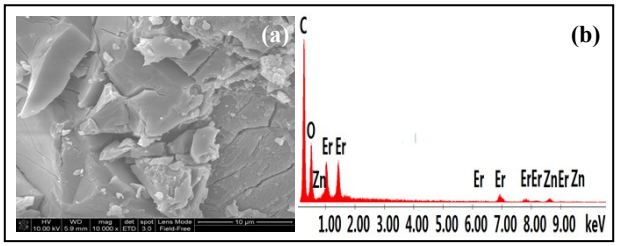


Figure S4. SEM image (a) and EDX spectrum (b) of **2**.

6. The thermogravimetric analysis of 1-2

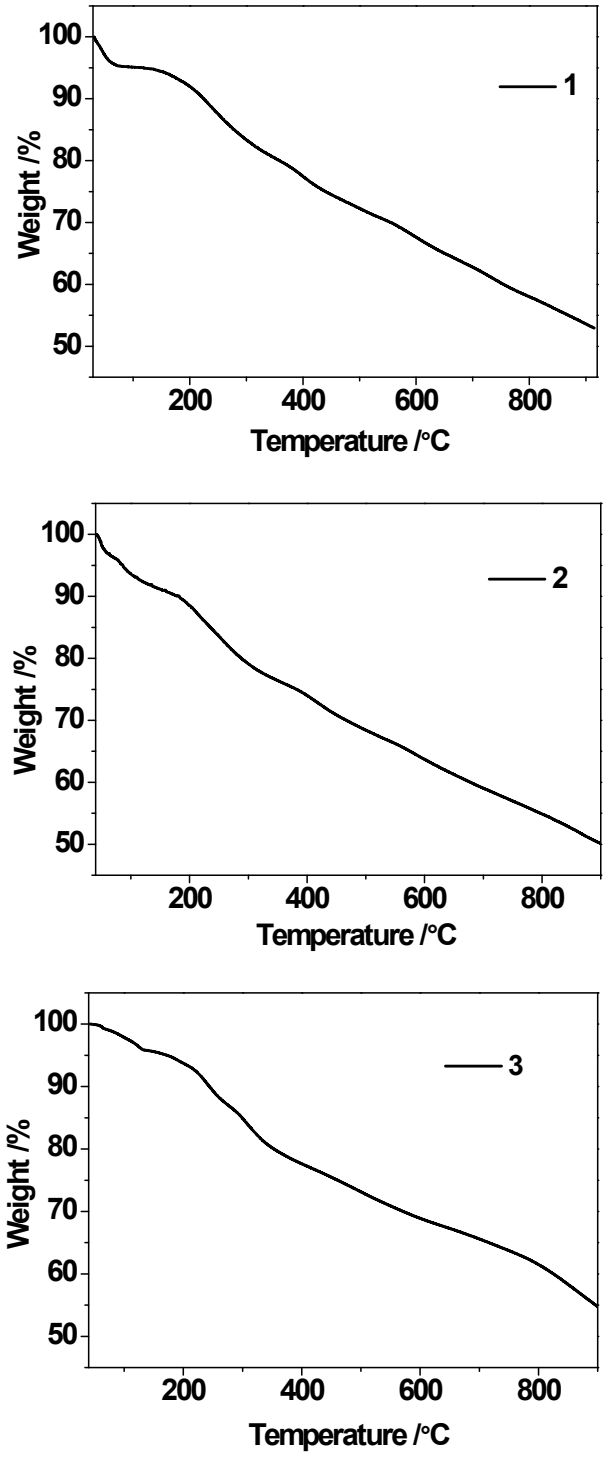


Figure S5. The thermogravimetric analysis of **1**-**3**.

7. Photophysical properties of the free ligands H_2L^1 and H_2L^2

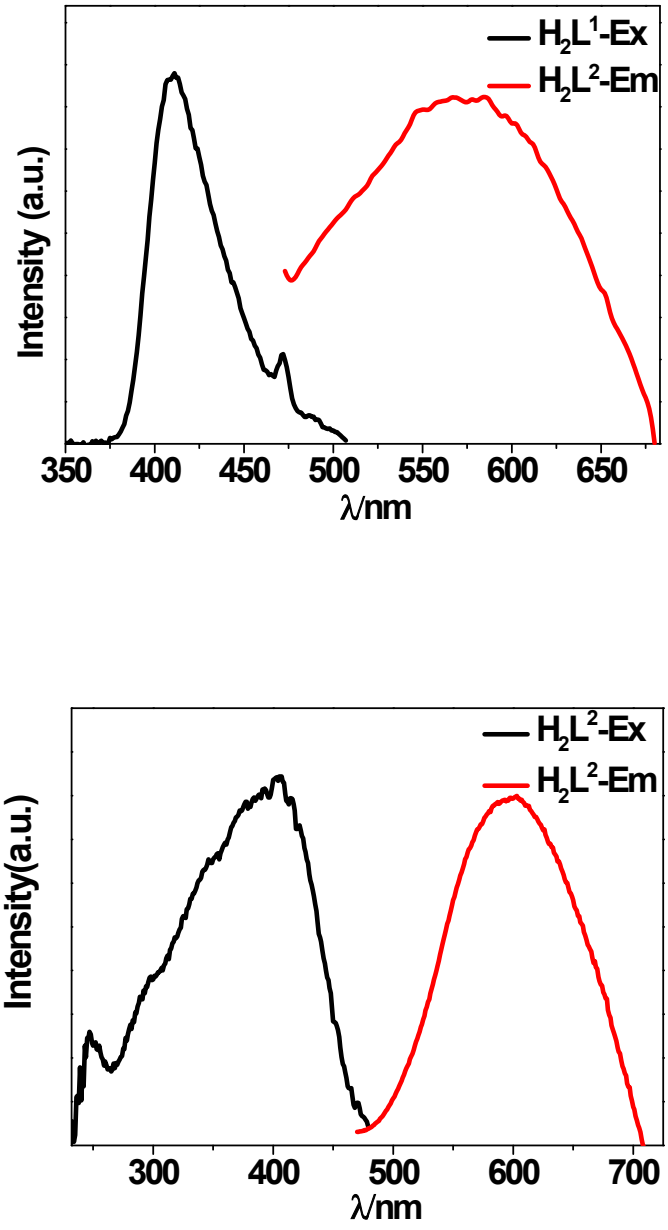


Figure S6. Photophysical properties of the free ligands H_2L^1 and H_2L^2 in CH_3CN.

8. The excitation and visible emission spectra of 1 and 3

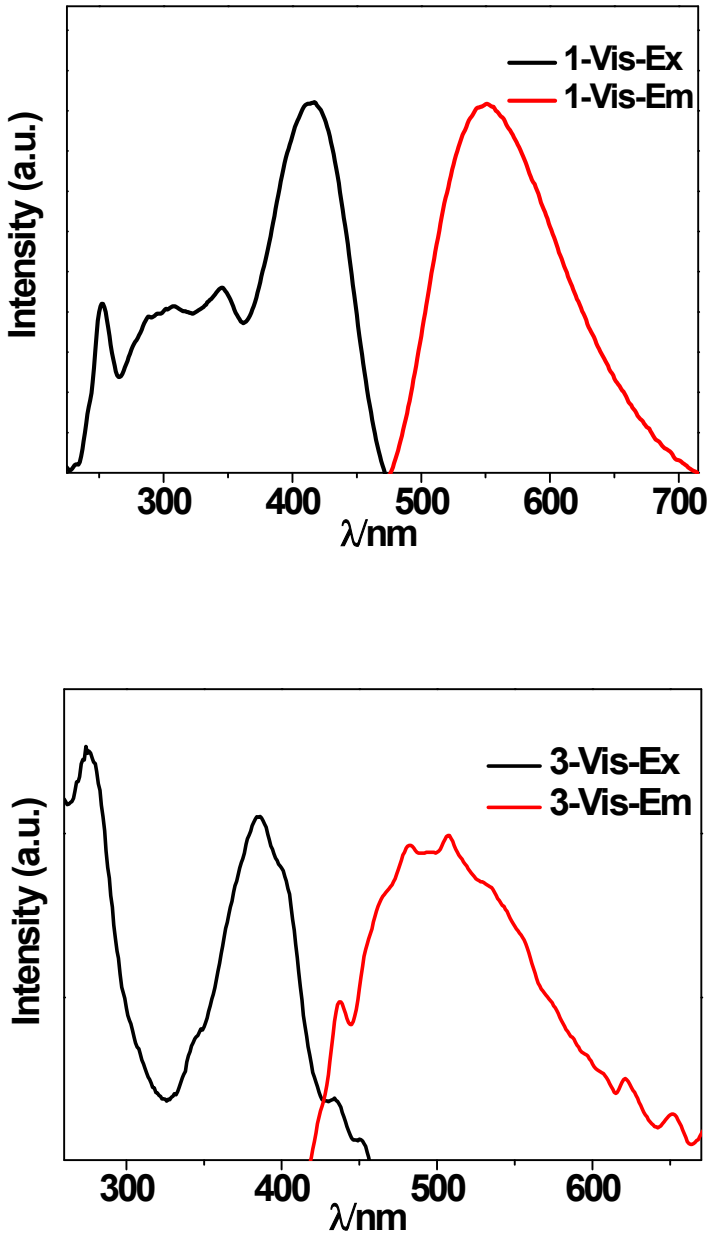


Figure S7. The excitation and visible emission spectra of **1** and **3** in CH_3CN.

9. The NIR emission lifetimes of 1-3

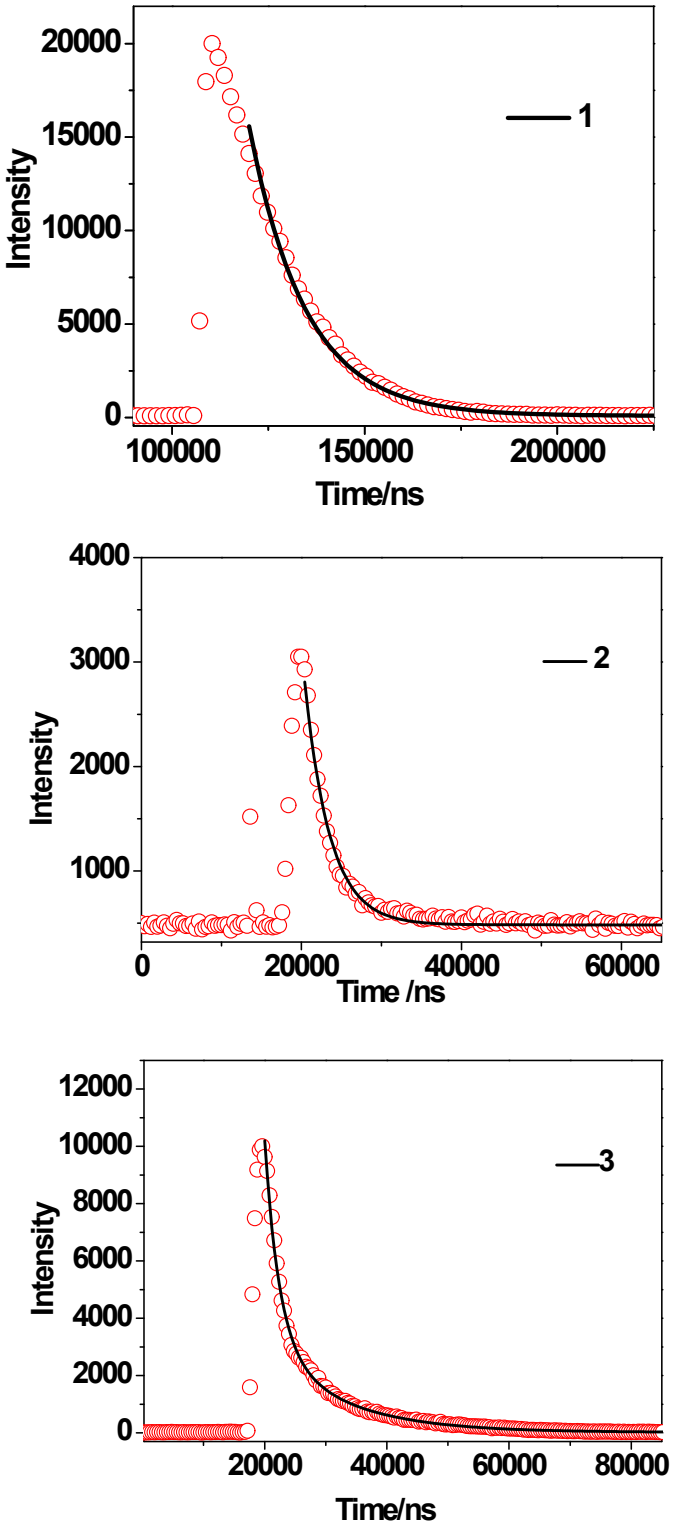
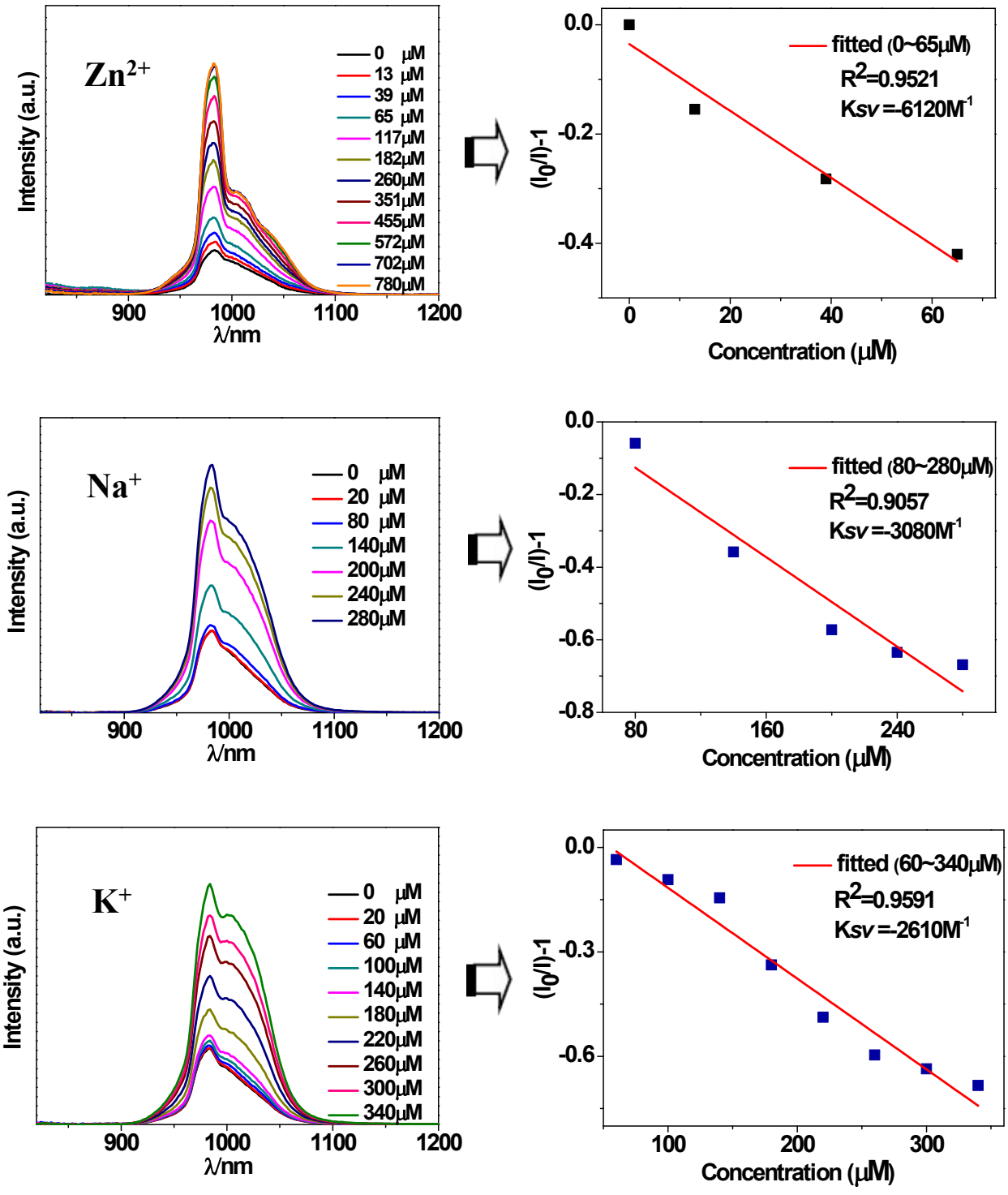
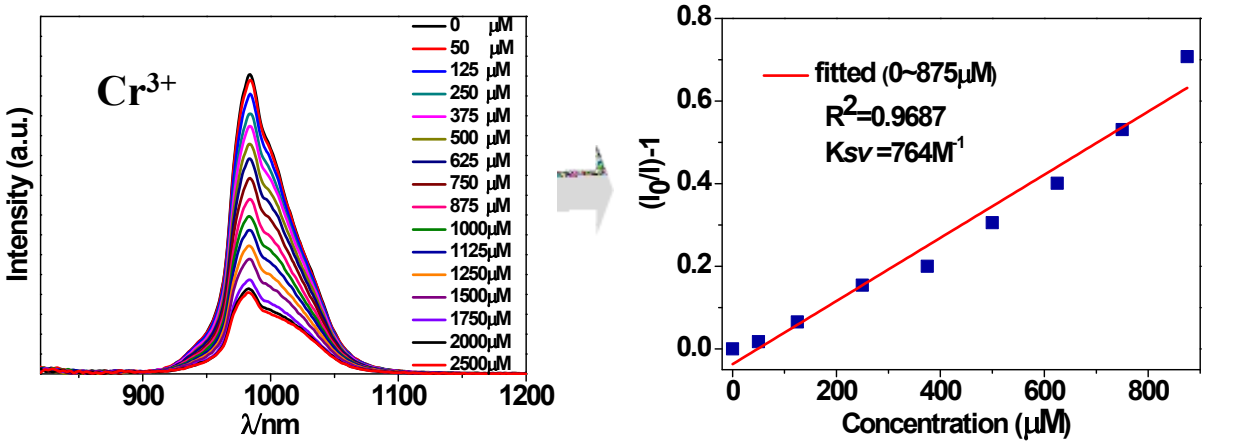
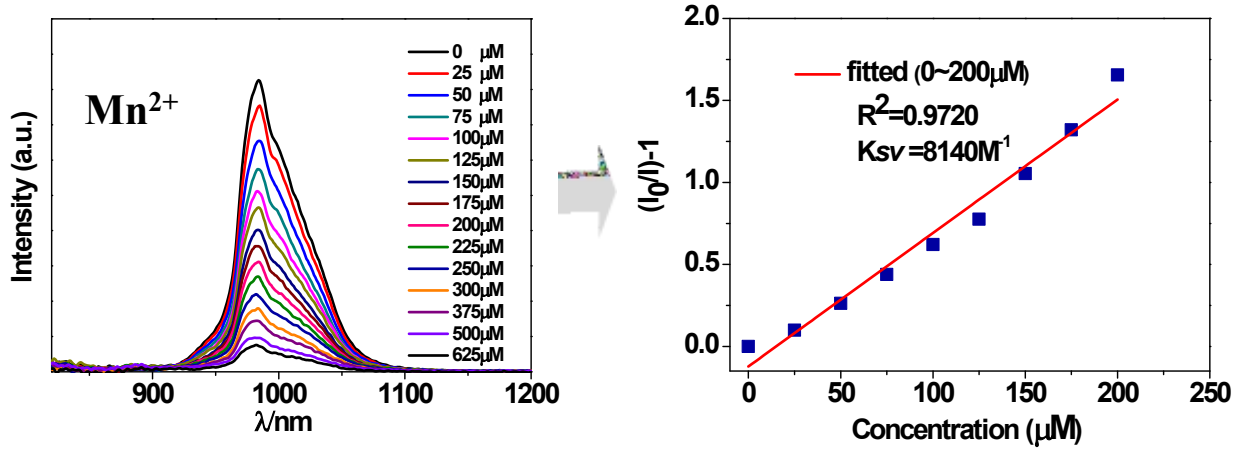


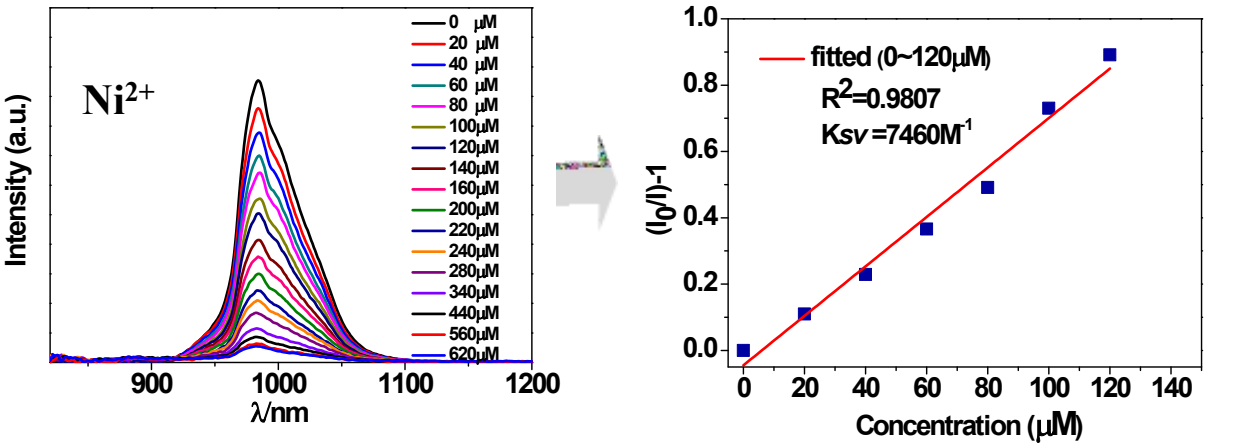
Figure S8. The NIR emission lifetimes of **1-3** in CH_3CN.

10. NIR luminescent sensing of 3 towards metal ions




Cr3+
Intensity (a.u.)
λ/nm
0 μM
50 μM
125 μM
250 μM
375 μM
500 μM
625 μM
750 μM
875 μM
1000μM
1125μM
1250μM
1500μM
1750μM
2000μM
2500μM
fitted (0~875μM)
R2=0.9687
Ksv =764M-1
(I0/I)-1
Concentration (μM)


Mn2+
Intensity (a.u.)
λ/nm
0 μM
25 μM
50 μM
75 μM
100μM
125μM
150μM
175μM
200μM
225μM
250μM
300μM
375μM
500μM
625μM
fitted (0~200μM)
R2=0.9720
Ksv =8140M-1
(I0/I)-1
Concentration (μM)


Ni2+
Intensity (a.u.)
λ/nm
0 μM
20 μM
40 μM
60 μM
80 μM
100μM
120μM
140μM
160μM
200μM
220μM
240μM
280μM
340μM
440μM
560μM
620μM
fitted (0~120μM)
R2=0.9807
Ksv =7460M-1
(I0/I)-1
Concentration (μM)

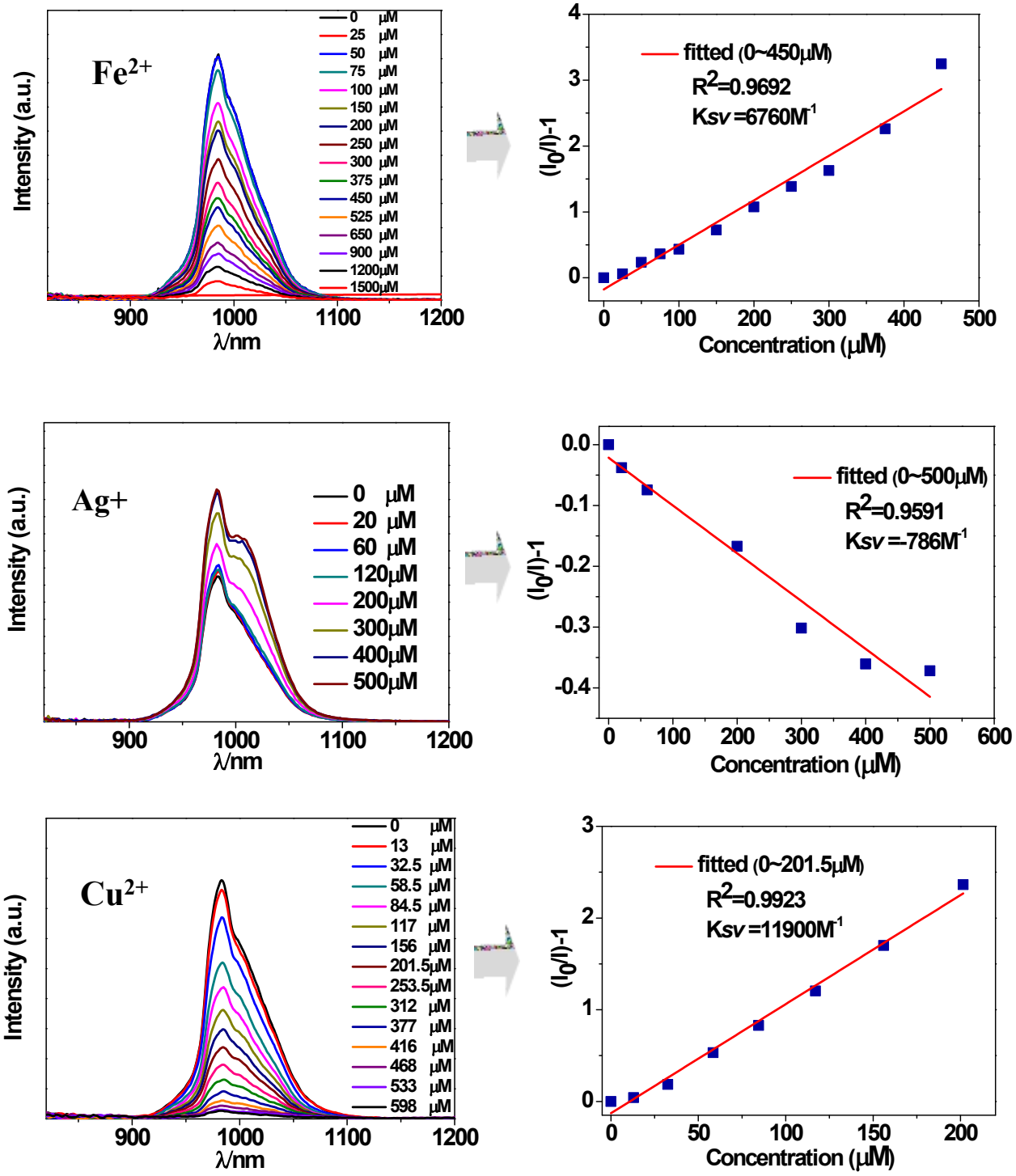


Figure S9. NIR luminescent sensing of **3** (60 μM) towards metal ions in DMF.

11. Visible emission response of 3 to metal ions

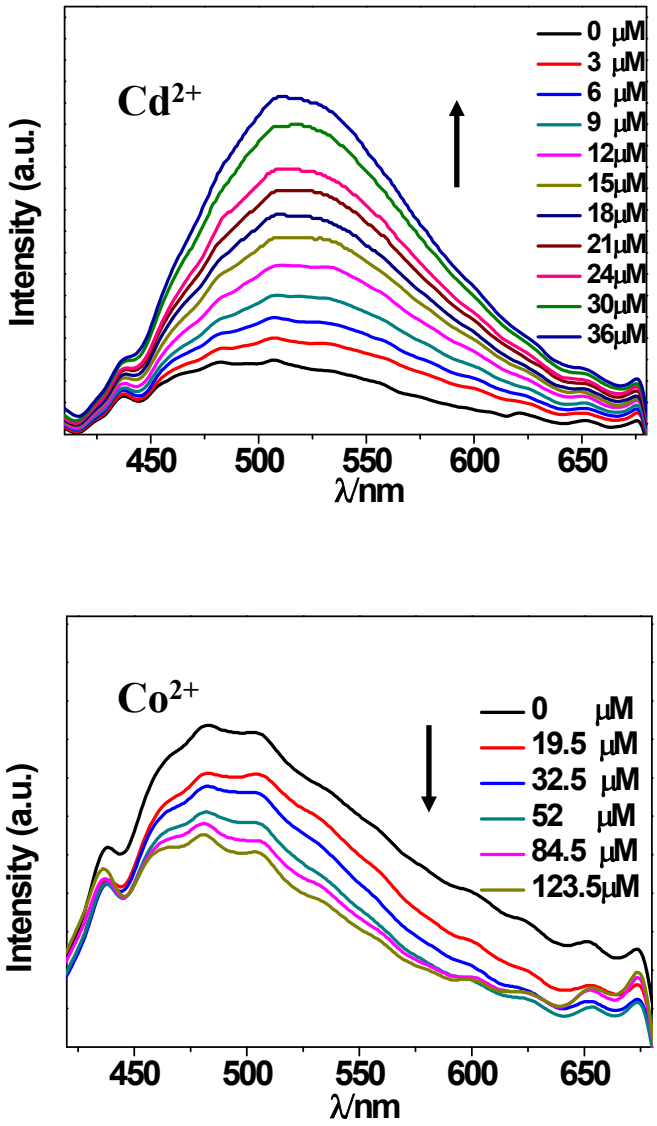


Figure S10. Visible emission response of **3** (60 μM) to metal ions in DMF.

12. X-Ray Crystallography

Data were collected on a Smart APEX CCD diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å) at 190 K. The data set was corrected for absorption based on multiple scans and reduced using standard methods. Data reduction was performed using DENZO-SMN.[1] The structures were solved by direct methods and refined anisotropically using full-matrix least-squares methods with the SHELX 97 program package.[2] Coordinates of the non-hydrogen atoms were refined anisotropically, while hydrogen atoms were included in the calculation isotropically but not refined. Neutral atom scattering factors were taken from Cromer and Waber.[3] Crystallographic data for **1-3** have been deposited with the Cambridge Crystallographic Data (CCDC reference numbers 1860701-1860703). These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif. Selected bond lengths and angles are given in Tables S1-S3.

(1) Otwinowski, Z.; Minor, W. DENZO-SMN. **1997**. *Methods in Enzymology*, *276*: *Macromolecular Crystallography, Part A*, 307−326, C. W. J. Carter, M. I. Simon and R. M. Sweet, Editors, Academic Press.

(2) Sheldrick, G. H. SHELX 97, *A software package for the solution and refinement of X-ray data*; University of Göttingen: Göttingen, Germany, **1997**.

(3) Cromer, D. T.; Waber, J. T. *International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham, **1974,** *4*, Table 2.2A.

Table S1. Selected bond lengths (Å) and angles (°) for **1**.

Yb(1)-O(2)	2.291(9)	O(7)-Yb(1)-O(6)	64.6(3)
Yb(1)-O(7)	2.297(9)	O(15)-Yb(1)-O(6)	78.9(4)
Yb(1)-O(15)	2.325(10)	O(12)-Yb(1)-O(6)	82.4(4)
Yb(1)-O(12)	2.353(11)	O(14)-Yb(1)-O(6)	130.2(3)
Yb(1)-O(14)	2.360(11)	O(11)-Yb(1)-O(6)	84.8(3)
Yb(1)-O(11)	2.409(10)	O(13)-Yb(1)-O(6)	76.5(4)
Yb(1)-O(13)	2.422(11)	O(2)-Yb(1)-O(1)	63.6(3)
Yb(1)-O(6)	2.472(12)	O(7)-Yb(1)-O(1)	117.9(3)
Yb(1)-O(1)	2.610(10)	O(15)-Yb(1)-O(1)	130.0(4)
Yb(2)-O(4)	2.304(9)	O(12)-Yb(1)-O(1)	72.7(3)
Yb(2)-O(9)	2.311(8)	O(14)-Yb(1)-O(1)	67.3(3)
Yb(2)-O(18)	2.312(8)	O(11)-Yb(1)-O(1)	68.8(3)
Yb(2)-O(21)	2.348(10)	O(13)-Yb(1)-O(1)	110.0(4)
Yb(2)-O(20)	2.369(10)	O(6)-Yb(1)-O(1)	151.1(3)
Yb(2)-O(19)	2.392(10)	O(4)-Yb(2)-O(9)	65.9(3)
Yb(2)-O(22)	2.439(9)	O(4)-Yb(2)-O(18)	74.7(3)
Yb(2)-O(5)	2.460(10)	O(9)-Yb(2)-O(18)	81.5(3)
Yb(2)-O(10)	2.595(10)	O(4)-Yb(2)-O(21)	121.4(3)
Zn(1)-O(16)	2.002(8)	O(9)-Yb(2)-O(21)	130.5(3)
Zn(1)-O(2)	2.015(9)	O(18)-Yb(2)-O(21)	147.0(3)
Zn(1)-N(1)	2.065(11)	O(4)-Yb(2)-O(20)	130.6(3)
Zn(1)-O(7)	2.090(9)	O(9)-Yb(2)-O(20)	142.4(3)
Zn(1)-N(3)	2.107(11)	O(18)-Yb(2)-O(20)	73.8(3)
Zn(2)-O(17)	1.985(8)	O(21)-Yb(2)-O(20)	74.6(3)
Zn(2)-O(9)	1.998(9)	O(4)-Yb(2)-O(19)	145.1(3)
Zn(2)-N(4)	2.056(9)	O(9)-Yb(2)-O(19)	92.7(3)
Zn(2)-O(4)	2.066(9)	O(18)-Yb(2)-O(19)	75.2(3)
Zn(2)-N(2)	2.086(12)	O(21)-Yb(2)-O(19)	93.4(4)
O(2)-Yb(1)-O(7)	66.7(3)	O(20)-Yb(2)-O(19)	54.0(3)
O(2)-Yb(1)-O(15)	82.4(3)	O(4)-Yb(2)-O(22)	76.1(3)
O(7)-Yb(1)-O(15)	74.4(3)	O(9)-Yb(2)-O(22)	87.9(3)
O(2)-Yb(1)-O(12)	131.8(4)	O(18)-Yb(2)-O(22)	150.7(3)
O(7)-Yb(1)-O(12)	123.0(4)	O(21)-Yb(2)-O(22)	53.8(3)
O(15)-Yb(1)-O(12)	144.6(4)	O(20)-Yb(2)-O(22)	126.6(3)
O(2)-Yb(1)-O(14)	87.3(3)	O(19)-Yb(2)-O(22)	132.8(3)
O(7)-Yb(1)-O(14)	142.7(3)	O(4)-Yb(2)-O(5)	64.8(3)
O(15)-Yb(1)-O(14)	76.1(4)	O(9)-Yb(2)-O(5)	130.4(3)
O(12)-Yb(1)-O(14)	94.1(4)	O(18)-Yb(2)-O(5)	81.2(3)
O(2)-Yb(1)-O(11)	90.9(3)	O(21)-Yb(2)-O(5)	81.3(4)
O(7)-Yb(1)-O(11)	77.3(3)	O(20)-Yb(2)-O(5)	73.6(3)
O(15)-Yb(1)-O(11)	151.3(4)	O(19)-Yb(2)-O(5)	126.5(3)
O(12)-Yb(1)-O(11)	53.6(4)	O(22)-Yb(2)-O(5)	85.1(3)
O(14)-Yb(1)-O(11)	131.7(4)	O(4)-Yb(2)-O(10)	118.5(3)
O(2)-Yb(1)-O(13)	137.5(4)	O(9)-Yb(2)-O(10)	63.4(3)
O(7)-Yb(1)-O(13)	131.8(4)	O(18)-Yb(2)-O(10)	127.1(3)
O(15)-Yb(1)-O(13)	71.0(3)	O(21)-Yb(2)-O(10)	73.5(3)
O(12)-Yb(1)-O(13)	75.5(4)	O(20)-Yb(2)-O(10)	110.8(3)
O(14)-Yb(1)-O(13)	54.9(4)	O(19)-Yb(2)-O(10)	68.7(3)
O(11)-Yb(1)-O(13)	127.7(4)	O(22)-Yb(2)-O(10)	69.6(3)
O(2)-Yb(1)-O(6)	130.8(3)	O(5)-Yb(2)-O(10)	151.6(3)

Table S2. Selected bond lengths (Å) and angles (°) for **2**.

Er(1)-O(2)	2.314(9)	O(7)-Er(1)-O(6)	62.6(4)
Er(1)-O(7)	2.358(11)	O(11)-Er(1)-O(6)	83.8(4)
Er(1)-O(11)	2.403(13)	O(15)-Er(1)-O(6)	79.3(4)
Er(1)-O(15)	2.407(11)	O(14)-Er(1)-O(6)	129.7(5)
Er(1)-O(14)	2.427(13)	O(12)-Er(1)-O(6)	83.2(4)
Er(1)-O(12)	2.430(10)	O(13)-Er(1)-O(6)	78.7(5)
Er(1)-O(13)	2.495(15)	O(2)-Er(1)-O(1)	63.0(3)
Er(1)-O(6)	2.564(11)	O(7)-Er(1)-O(1)	118.0(4)
Er(1)-O(1)	2.611(9)	O(11)-Er(1)-O(1)	70.3(4)
Er(2)-O(18)	2.330(11)	O(15)-Er(1)-O(1)	128.4(4)
Er(2)-O(9)	2.338(9)	O(14)-Er(1)-O(1)	69.4(4)
Er(2)-O(20)	2.356(13)	O(12)-Er(1)-O(1)	73.6(3)
Er(2)-O(4)	2.359(9)	O(13)-Er(1)-O(1)	110.2(4)
Er(2)-O(22)	2.425(12)	O(6)-Er(1)-O(1)	152.1(4)
Er(2)-O(21)	2.437(11)	O(18)-Er(2)-O(9)	80.5(4)
Er(2)-O(19)	2.464(11)	O(18)-Er(2)-O(20)	74.9(4)
Er(2)-O(5)	2.547(10)	O(9)-Er(2)-O(20)	139.6(3)
Er(2)-O(10)	2.678(9)	O(18)-Er(2)-O(4)	73.2(4)
Zn(1)-O(16)	1.985(11)	O(9)-Er(2)-O(4)	67.0(3)
Zn(1)-O(2)	2.027(9)	O(20)-Er(2)-O(4)	132.0(3)
Zn(1)-N(1)	2.089(10)	O(18)-Er(2)-O(22)	149.7(4)
Zn(1)-N(3)	2.101(12)	O(9)-Er(2)-O(22)	89.3(4)
Zn(1)-O(7)	2.128(9)	O(20)-Er(2)-O(22)	126.9(4)
Zn(2)-O(17)	1.962(11)	O(4)-Er(2)-O(22)	76.5(4)
Zn(2)-O(9)	2.018(8)	O(18)-Er(2)-O(21)	146.3(5)
Zn(2)-N(4)	2.096(10)	O(9)-Er(2)-O(21)	132.4(4)
Zn(2)-O(4)	2.099(8)	O(20)-Er(2)-O(21)	73.6(5)
Zn(2)-N(2)	2.096(12)	O(4)-Er(2)-O(21)	121.7(4)
O(2)-Er(1)-O(7)	67.5(3)	O(22)-Er(2)-O(21)	54.4(5)
O(2)-Er(1)-O(11)	91.0(4)	O(18)-Er(2)-O(19)	77.2(4)
O(7)-Er(1)-O(11)	75.8(4)	O(9)-Er(2)-O(19)	90.9(4)
O(2)-Er(1)-O(15)	80.1(4)	O(20)-Er(2)-O(19)	52.9(3)
O(7)-Er(1)-O(15)	73.1(4)	O(4)-Er(2)-O(19)	145.4(3)
O(11)-Er(1)-O(15)	148.7(4)	O(22)-Er(2)-O(19)	131.7(4)
O(2)-Er(1)-O(14)	86.6(4)	O(21)-Er(2)-O(19)	92.9(4)
O(7)-Er(1)-O(14)	141.0(4)	O(18)-Er(2)-O(5)	78.2(4)
O(11)-Er(1)-O(14)	135.8(4)	O(9)-Er(2)-O(5)	129.5(3)
O(15)-Er(1)-O(14)	74.0(4)	O(20)-Er(2)-O(5)	75.9(4)
O(2)-Er(1)-O(12)	132.3(4)	O(4)-Er(2)-O(5)	63.2(3)
O(7)-Er(1)-O(12)	122.6(4)	O(22)-Er(2)-O(5)	86.9(4)
O(11)-Er(1)-O(12)	54.8(5)	O(21)-Er(2)-O(5)	82.9(3)
O(15)-Er(1)-O(12)	146.5(5)	O(19)-Er(2)-O(5)	127.2(4)
O(14)-Er(1)-O(12)	96.4(4)	O(18)-Er(2)-O(10)	126.9(3)
O(2)-Er(1)-O(13)	134.8(4)	O(9)-Er(2)-O(10)	61.8(3)
O(7)-Er(1)-O(13)	131.1(4)	O(20)-Er(2)-O(10)	110.2(3)
O(11)-Er(1)-O(13)	130.7(5)	O(4)-Er(2)-O(10)	117.5(3)
O(15)-Er(1)-O(13)	71.2(4)	O(22)-Er(2)-O(10)	69.8(3)
O(14)-Er(1)-O(13)	52.6(4)	O(21)-Er(2)-O(10)	75.9(3)
O(12)-Er(1)-O(13)	77.5(5)	O(19)-Er(2)-O(10)	68.0(4)
O(2)-Er(1)-O(6)	129.6(4)	O(5)-Er(2)-O(10)	154.9(3)

Table S3. Selected bond lengths (Å) and angles (°) for **3**.

Yb(1)-O(22)	2.377(12)	Yb(7)-O(36)	2.320(16)
Yb(1)-O(27)	2.382(13)	Yb(7)-O(30)	2.344(13)
Yb(1)-O(34)	2.383(12)	Yb(7)-O(51)	2.362(12)
Yb(1)-O(50)	2.389(11)	Yb(7)-O(35)	2.374(13)
Yb(1)-O(35)	2.410(12)	Yb(7)-O(50)	2.403(12)
Yb(1)-O(33)	2.416(11)	Yb(7)-O(46)	2.407(14)
Yb(1)-O(31)	2.445(12)	Yb(7)-O(11)	2.438(13)
Yb(1)-O(20)	2.492(12)	Yb(7)-O(49)	2.466(14)
Yb(2)-O(43)	2.328(12)	Yb(8)-O(51)	2.371(12)
Yb(2)-O(2)	2.379(12)	Yb(8)-O(13)	2.402(18)
Yb(2)-O(41)	2.387(13)	Yb(8)-O(8)	2.403(16)
Yb(2)-O(6)	2.393(12)	Yb(8)-O(47)	2.419(15)
Yb(2)-O(33)	2.399(11)	Yb(8)-O(10)	2.479(17)
Yb(2)-O(34)	2.493(11)	Yb(8)-O(45)	2.482(15)
Yb(2)-O(42)	2.524(15)	Yb(8)-O(9)	2.500(17)
Yb(2)-N(1)	2.600(17)	Yb(8)-O(11)	2.568(15)
Yb(2)-O(7)	2.701(16)	Yb(8)-O(14)	2.655(14)
Yb(3)-O(18)	2.361(13)	Yb(9)-O(3)	2.286(17)
Yb(3)-O(16)	2.376(13)	Yb(9)-O(31)	2.361(12)
Yb(3)-O(51)	2.397(12)	Yb(9)-O(48)	2.362(16)
Yb(3)-O(12)	2.418(17)	Yb(9)-O(38)	2.377(15)
Yb(3)-O(20)	2.481(12)	Yb(9)-O(30)	2.408(15)
Yb(3)-O(22)	2.500(12)	Yb(9)-O(29)	2.415(18)
Yb(3)-O(14)	2.506(13)	Yb(9)-O(35)	2.440(11)
Yb(3)-O(21)	2.567(16)	Yb(9)-O(4)	2.619(17)
Yb(3)-O(13)	2.788(16)	O(22)-Yb(1)-O(27)	81.4(4)
Yb(4)-O(20)	2.362(12)	O(22)-Yb(1)-O(34)	143.8(4)
Yb(4)-O(15)	2.367(16)	O(27)-Yb(1)-O(34)	80.2(4)
Yb(4)-O(33)	2.375(11)	O(22)-Yb(1)-O(50)	131.5(4)
Yb(4)-O(40)	2.422(16)	O(27)-Yb(1)-O(50)	141.5(4)
Yb(4)-O(2)	2.455(13)	O(34)-Yb(1)-O(50)	79.5(4)
Yb(4)-O(19)	2.466(14)	O(22)-Yb(1)-O(35)	74.2(4)
Yb(4)-O(18)	2.534(13)	O(27)-Yb(1)-O(35)	112.5(4)
Yb(4)-O(1)	2.603(13)	O(34)-Yb(1)-O(35)	141.9(4)
Yb(4)-O(41)	2.609(14)	O(50)-Yb(1)-O(35)	68.6(4)
Yb(5)-O(31)	2.324(11)	O(22)-Yb(1)-O(33)	74.4(4)
Yb(5)-O(37)	2.334(14)	O(27)-Yb(1)-O(33)	81.4(4)
Yb(5)-O(39)	2.384(15)	O(34)-Yb(1)-O(33)	72.1(4)
Yb(5)-O(25)	2.406(13)	O(50)-Yb(1)-O(33)	122.1(4)
Yb(5)-O(50)	2.434(11)	O(35)-Yb(1)-O(33)	143.1(4)
Yb(5)-O(30)	2.450(15)	O(22)-Yb(1)-O(31)	124.2(4)
Yb(5)-O(24)	2.467(12)	O(27)-Yb(1)-O(31)	77.6(4)
Yb(5)-O(32)	2.484(15)	O(34)-Yb(1)-O(31)	81.5(4)
Yb(6)-O(34)	2.371(12)	O(50)-Yb(1)-O(31)	67.3(4)
Yb(6)-O(5)	2.391(13)	O(35)-Yb(1)-O(31)	67.6(4)
Yb(6)-O(6)	2.444(13)	O(33)-Yb(1)-O(31)	148.6(4)
Yb(6)-O(28)	2.449(16)	O(22)-Yb(1)-O(20)	68.8(4)
Yb(6)-O(23)	2.450(13)	O(27)-Yb(1)-O(20)	141.8(4)
Yb(6)-O(26)	2.456(14)	O(34)-Yb(1)-O(20)	110.2(4)
Yb(6)-O(43)	2.467(12)	O(50)-Yb(1)-O(20)	76.3(4)
Yb(6)-O(24)	2.559(12)	O(35)-Yb(1)-O(20)	82.4(4)
Yb(6)-O(44)	2.664(14)	O(33)-Yb(1)-O(20)	68.3(4)

O(31)-Yb(1)-O(20)	139.1(4)	O(12)-Yb(3)-O(14)	79.5(5)
O(43)-Yb(2)-O(2)	143.6(4)	O(20)-Yb(3)-O(14)	76.0(4)
O(43)-Yb(2)-O(41)	99.7(5)	O(22)-Yb(3)-O(14)	141.8(4)
O(2)-Yb(2)-O(41)	74.4(5)	O(18)-Yb(3)-O(21)	71.6(5)
O(43)-Yb(2)-O(6)	67.0(4)	O(16)-Yb(3)-O(21)	72.0(5)
O(2)-Yb(2)-O(6)	140.3(5)	O(51)-Yb(3)-O(21)	140.5(5)
O(41)-Yb(2)-O(6)	136.6(4)	O(12)-Yb(3)-O(21)	78.4(5)
O(43)-Yb(2)-O(33)	141.6(4)	O(20)-Yb(3)-O(21)	114.0(4)
O(2)-Yb(2)-O(33)	70.7(4)	O(22)-Yb(3)-O(21)	52.4(4)
O(41)-Yb(2)-O(33)	68.8(4)	O(14)-Yb(3)-O(21)	146.4(5)
O(6)-Yb(2)-O(33)	95.7(4)	O(18)-Yb(3)-O(13)	124.8(5)
O(43)-Yb(2)-O(34)	71.4(4)	O(16)-Yb(3)-O(13)	77.1(5)
O(2)-Yb(2)-O(34)	132.6(4)	O(51)-Yb(3)-O(13)	65.1(5)
O(41)-Yb(2)-O(34)	66.8(4)	O(12)-Yb(3)-O(13)	50.0(5)
O(6)-Yb(2)-O(34)	69.9(4)	O(20)-Yb(3)-O(13)	127.2(5)
O(33)-Yb(2)-O(34)	70.5(4)	O(22)-Yb(3)-O(13)	153.8(4)
O(43)-Yb(2)-O(42)	71.3(5)	O(14)-Yb(3)-O(13)	61.1(5)
O(2)-Yb(2)-O(42)	72.9(5)	O(21)-Yb(3)-O(13)	118.8(5)
O(41)-Yb(2)-O(42)	70.6(5)	O(20)-Yb(4)-O(15)	81.1(5)
O(6)-Yb(2)-O(42)	132.9(5)	O(20)-Yb(4)-O(33)	71.2(4)
O(33)-Yb(2)-O(42)	131.0(4)	O(15)-Yb(4)-O(33)	149.7(5)
O(34)-Yb(2)-O(42)	115.9(4)	O(20)-Yb(4)-O(40)	89.3(5)
O(43)-Yb(2)-N(1)	90.5(5)	O(15)-Yb(4)-O(40)	73.4(6)
O(2)-Yb(2)-N(1)	73.2(5)	O(33)-Yb(4)-O(40)	117.0(4)
O(41)-Yb(2)-N(1)	137.5(5)	O(20)-Yb(4)-O(2)	137.0(4)
O(6)-Yb(2)-N(1)	85.3(5)	O(15)-Yb(4)-O(2)	140.2(5)
O(33)-Yb(2)-N(1)	123.3(5)	O(33)-Yb(4)-O(2)	69.9(4)
O(34)-Yb(2)-N(1)	153.4(5)	O(40)-Yb(4)-O(2)	92.5(5)
O(42)-Yb(2)-N(1)	74.0(5)	O(20)-Yb(4)-O(19)	121.2(5)
O(43)-Yb(2)-O(7)	123.1(4)	O(15)-Yb(4)-O(19)	91.3(6)
O(2)-Yb(2)-O(7)	80.1(5)	O(33)-Yb(4)-O(19)	92.8(5)
O(41)-Yb(2)-O(7)	133.5(5)	O(40)-Yb(4)-O(19)	143.8(5)
O(6)-Yb(2)-O(7)	60.5(4)	O(2)-Yb(4)-O(19)	78.3(5)
O(33)-Yb(2)-O(7)	66.2(4)	O(20)-Yb(4)-O(18)	72.1(4)
O(34)-Yb(2)-O(7)	107.7(4)	O(15)-Yb(4)-O(18)	71.5(5)
O(42)-Yb(2)-O(7)	136.3(5)	O(33)-Yb(4)-O(18)	88.3(4)
N(1)-Yb(2)-O(7)	65.5(5)	O(40)-Yb(4)-O(18)	142.3(5)
O(18)-Yb(3)-O(16)	143.4(5)	O(2)-Yb(4)-O(18)	123.6(4)
O(18)-Yb(3)-O(51)	142.1(4)	O(19)-Yb(4)-O(18)	50.7(4)
O(16)-Yb(3)-O(51)	71.1(5)	O(20)-Yb(4)-O(1)	156.6(4)
O(18)-Yb(3)-O(12)	86.1(5)	O(15)-Yb(4)-O(1)	78.1(5)
O(16)-Yb(3)-O(12)	90.0(6)	O(33)-Yb(4)-O(1)	131.3(4)
O(51)-Yb(3)-O(12)	115.0(5)	O(40)-Yb(4)-O(1)	74.6(5)
O(18)-Yb(3)-O(20)	73.0(4)	O(2)-Yb(4)-O(1)	62.2(4)
O(16)-Yb(3)-O(20)	119.8(5)	O(19)-Yb(4)-O(1)	70.2(5)
O(51)-Yb(3)-O(20)	74.0(4)	O(18)-Yb(4)-O(1)	110.7(4)
O(12)-Yb(3)-O(20)	149.7(5)	O(20)-Yb(4)-O(41)	78.6(4)
O(18)-Yb(3)-O(22)	78.5(4)	O(15)-Yb(4)-O(41)	121.1(5)
O(16)-Yb(3)-O(22)	76.7(5)	O(33)-Yb(4)-O(41)	65.5(4)
O(51)-Yb(3)-O(22)	105.1(4)	O(40)-Yb(4)-O(41)	51.9(4)
O(12)-Yb(3)-O(22)	130.8(5)	O(2)-Yb(4)-O(41)	69.3(4)
O(20)-Yb(3)-O(22)	67.1(4)	O(19)-Yb(4)-O(41)	145.5(5)
O(18)-Yb(3)-O(14)	81.9(5)	O(18)-Yb(4)-O(41)	145.8(4)
O(16)-Yb(3)-O(14)	133.0(5)	O(1)-Yb(4)-O(41)	103.2(4)
O(51)-Yb(3)-O(14)	72.4(4)	O(31)-Yb(5)-O(37)	143.9(5)

O(31)-Yb(5)-O(39)	87.9(5)	O(34)-Yb(6)-O(44)	129.7(4)
O(37)-Yb(5)-O(39)	95.5(6)	O(5)-Yb(6)-O(44)	71.4(5)
O(31)-Yb(5)-O(25)	109.7(4)	O(6)-Yb(6)-O(44)	101.9(4)
O(37)-Yb(5)-O(25)	86.9(5)	O(28)-Yb(6)-O(44)	146.3(5)
O(39)-Yb(5)-O(25)	146.1(5)	O(23)-Yb(6)-O(44)	80.3(5)
O(31)-Yb(5)-O(50)	68.5(4)	O(26)-Yb(6)-O(44)	65.2(5)
O(37)-Yb(5)-O(50)	87.5(5)	O(43)-Yb(6)-O(44)	61.9(4)
O(39)-Yb(5)-O(50)	140.9(5)	O(24)-Yb(6)-O(44)	117.9(4)
O(25)-Yb(5)-O(50)	73.0(4)	O(36)-Yb(7)-O(30)	77.6(6)
O(31)-Yb(5)-O(30)	69.2(5)	O(36)-Yb(7)-O(51)	143.6(5)
O(37)-Yb(5)-O(30)	77.1(5)	O(30)-Yb(7)-O(51)	137.8(5)
O(39)-Yb(5)-O(30)	74.7(5)	O(36)-Yb(7)-O(35)	142.9(5)
O(25)-Yb(5)-O(30)	138.2(4)	O(30)-Yb(7)-O(35)	68.3(5)
O(50)-Yb(5)-O(30)	68.0(4)	O(51)-Yb(7)-O(35)	73.1(4)
O(31)-Yb(5)-O(24)	69.4(4)	O(36)-Yb(7)-O(50)	86.4(5)
O(37)-Yb(5)-O(24)	146.7(5)	O(30)-Yb(7)-O(50)	70.3(4)
O(39)-Yb(5)-O(24)	82.4(5)	O(51)-Yb(7)-O(50)	110.8(4)
O(25)-Yb(5)-O(24)	77.5(4)	O(35)-Yb(7)-O(50)	68.9(4)
O(50)-Yb(5)-O(24)	114.9(4)	O(36)-Yb(7)-O(46)	80.5(6)
O(30)-Yb(5)-O(24)	132.9(4)	O(30)-Yb(7)-O(46)	135.4(5)
O(31)-Yb(5)-O(32)	140.7(5)	O(51)-Yb(7)-O(46)	76.2(5)
O(37)-Yb(5)-O(32)	73.5(6)	O(35)-Yb(7)-O(46)	114.1(5)
O(39)-Yb(5)-O(32)	73.1(6)	O(50)-Yb(7)-O(46)	70.1(4)
O(25)-Yb(5)-O(32)	75.2(5)	O(36)-Yb(7)-O(11)	76.7(5)
O(50)-Yb(5)-O(32)	143.6(5)	O(30)-Yb(7)-O(11)	134.8(5)
O(30)-Yb(5)-O(32)	133.3(5)	O(51)-Yb(7)-O(11)	70.5(5)
O(24)-Yb(5)-O(32)	74.2(5)	O(35)-Yb(7)-O(11)	138.9(5)
O(34)-Yb(6)-O(5)	139.8(4)	O(50)-Yb(7)-O(11)	143.0(4)
O(34)-Yb(6)-O(6)	71.1(4)	O(46)-Yb(7)-O(11)	74.8(5)
O(5)-Yb(6)-O(6)	70.9(4)	O(36)-Yb(7)-O(49)	111.2(5)
O(34)-Yb(6)-O(28)	81.3(4)	O(30)-Yb(7)-O(49)	82.9(5)
O(5)-Yb(6)-O(28)	75.6(5)	O(51)-Yb(7)-O(49)	73.8(5)
O(6)-Yb(6)-O(28)	73.2(4)	O(35)-Yb(7)-O(49)	79.4(4)
O(34)-Yb(6)-O(23)	135.3(4)	O(50)-Yb(7)-O(49)	144.1(4)
O(5)-Yb(6)-O(23)	74.9(5)	O(46)-Yb(7)-O(49)	141.5(5)
O(6)-Yb(6)-O(23)	142.8(4)	O(11)-Yb(7)-O(49)	72.8(5)
O(28)-Yb(6)-O(23)	84.6(5)	O(51)-Yb(8)-O(13)	72.1(5)
O(34)-Yb(6)-O(26)	84.9(4)	O(51)-Yb(8)-O(8)	153.0(5)
O(5)-Yb(6)-O(26)	132.7(5)	O(13)-Yb(8)-O(8)	94.1(6)
O(6)-Yb(6)-O(26)	135.2(4)	O(51)-Yb(8)-O(47)	90.7(5)
O(28)-Yb(6)-O(26)	140.8(5)	O(13)-Yb(8)-O(47)	135.1(5)
O(23)-Yb(6)-O(26)	79.9(5)	O(8)-Yb(8)-O(47)	82.9(6)
O(34)-Yb(6)-O(43)	71.1(4)	O(51)-Yb(8)-O(10)	119.4(5)
O(5)-Yb(6)-O(43)	103.1(5)	O(13)-Yb(8)-O(10)	150.1(6)
O(6)-Yb(6)-O(43)	64.1(4)	O(8)-Yb(8)-O(10)	84.2(6)
O(28)-Yb(6)-O(43)	134.6(4)	O(47)-Yb(8)-O(10)	74.5(5)
O(23)-Yb(6)-O(43)	139.9(5)	O(51)-Yb(8)-O(45)	75.6(5)
O(26)-Yb(6)-O(43)	72.6(5)	O(13)-Yb(8)-O(45)	79.2(6)
O(34)-Yb(6)-O(24)	84.0(4)	O(8)-Yb(8)-O(45)	125.6(6)
O(5)-Yb(6)-O(24)	118.7(4)	O(47)-Yb(8)-O(45)	137.4(6)
O(6)-Yb(6)-O(24)	140.2(4)	O(10)-Yb(8)-O(45)	77.7(6)
O(28)-Yb(6)-O(24)	72.6(4)	O(51)-Yb(8)-O(9)	139.8(5)
O(23)-Yb(6)-O(24)	51.3(4)	O(13)-Yb(8)-O(9)	77.0(6)
O(26)-Yb(6)-O(24)	69.6(4)	O(8)-Yb(8)-O(9)	52.4(6)
O(43)-Yb(6)-O(24)	136.1(4)	O(47)-Yb(8)-O(9)	129.6(5)

O(10)-Yb(8)-O(9)	78.5(6)	O(3)-Yb(9)-O(30)	130.0(5)
O(45)-Yb(8)-O(9)	73.7(5)	O(31)-Yb(9)-O(30)	69.4(4)
O(51)-Yb(8)-O(11)	68.1(4)	O(48)-Yb(9)-O(30)	80.7(5)
O(13)-Yb(8)-O(11)	132.1(5)	O(38)-Yb(9)-O(30)	76.1(5)
O(8)-Yb(8)-O(11)	132.6(6)	O(3)-Yb(9)-O(29)	80.0(6)
O(47)-Yb(8)-O(11)	71.2(5)	O(31)-Yb(9)-O(29)	102.9(5)
O(10)-Yb(8)-O(11)	51.4(5)	O(48)-Yb(9)-O(29)	87.7(6)
O(45)-Yb(8)-O(11)	66.3(5)	O(38)-Yb(9)-O(29)	142.0(6)
O(9)-Yb(8)-O(11)	120.1(5)	O(30)-Yb(9)-O(29)	140.7(5)
O(51)-Yb(8)-O(14)	70.2(4)	O(3)-Yb(9)-O(35)	128.6(5)
O(13)-Yb(8)-O(14)	64.4(5)	O(31)-Yb(9)-O(35)	68.4(4)
O(8)-Yb(8)-O(14)	83.0(5)	O(48)-Yb(9)-O(35)	81.7(5)
O(47)-Yb(8)-O(14)	70.8(5)	O(38)-Yb(9)-O(35)	142.3(5)
O(10)-Yb(8)-O(14)	144.2(5)	O(30)-Yb(9)-O(35)	66.2(5)
O(45)-Yb(8)-O(14)	135.8(5)	O(29)-Yb(9)-O(35)	75.1(5)
O(9)-Yb(8)-O(14)	117.9(5)	O(3)-Yb(9)-O(4)	64.1(6)
O(11)-Yb(8)-O(14)	121.9(4)	O(31)-Yb(9)-O(4)	138.6(5)
O(3)-Yb(9)-O(31)	74.6(5)	O(48)-Yb(9)-O(4)	77.4(5)
O(3)-Yb(9)-O(48)	141.4(5)	O(38)-Yb(9)-O(4)	70.1(6)
O(31)-Yb(9)-O(48)	144.0(5)	O(30)-Yb(9)-O(4)	138.8(6)
O(3)-Yb(9)-O(38)	77.4(6)	O(29)-Yb(9)-O(4)	72.7(6)
O(31)-Yb(9)-O(38)	100.0(5)	O(35)-Yb(9)-O(4)	141.9(5)
O(48)-Yb(9)-O(38)	91.2(6)		